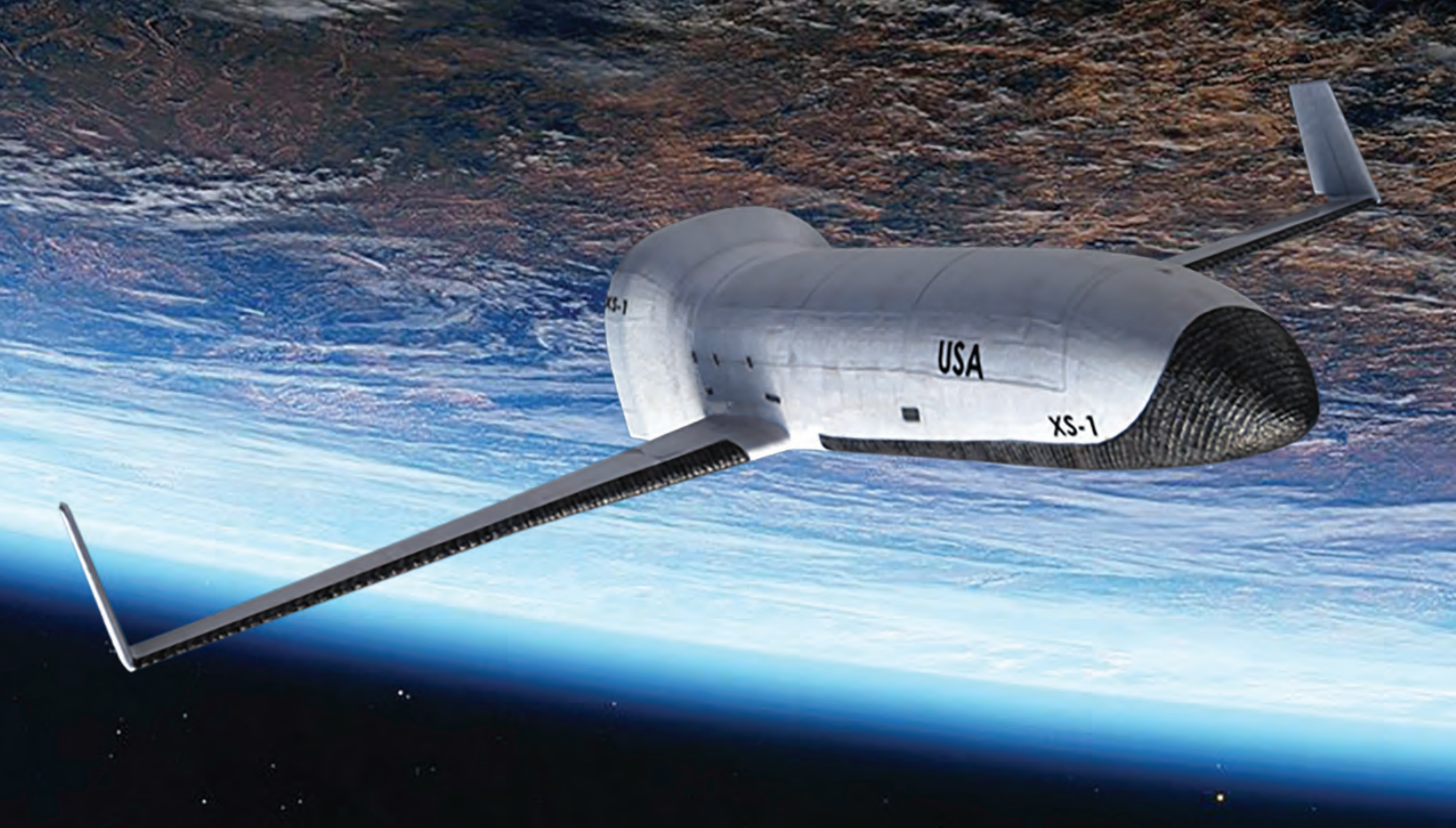
Lawrence Livermore National Laboratory

October/November 2015

Science & Technology REVIEW



BOOSTING AMERICA'S SPACE-LAUNCH INDUSTRY

Also in this issue:

X-Ray Optics Peer into Invisible Realms

A Two-Step Approach to Microbial Detection

Tailoring Reactive Materials

About the Cover

For more than two decades, Livermore researchers have pioneered the use of advanced simulation software and some of the world's most powerful supercomputers to virtually design, prototype, and test new components—and entire engineering systems—for national security missions. As the article beginning on p. 4 describes, Livermore engineers have recently developed new simulation tools and techniques for designing novel, cost-effective rocket engines and space-launch vehicles as part of two projects for the Defense Advanced Research Projects Agency. In one of these efforts, simulations were used to study the thermal and structural response of a candidate launch-vehicle design for the agency's proposed medium-lift-capacity XS-1 space plane. The artist's rendering on the cover depicts the a conceptual XS-1 flying in low-Earth orbit.

Cover design: Tom Reason; Rendering: Adam S. Connell

About *S&TR*

At Lawrence Livermore National Laboratory, we focus on science and technology research to ensure our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published eight times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

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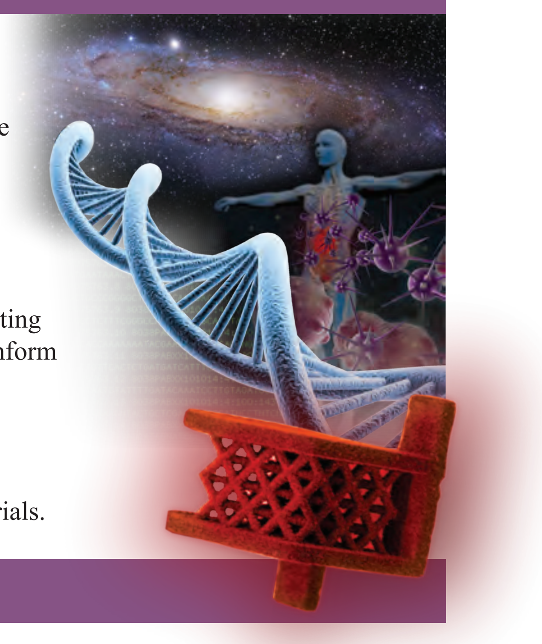
Feature

Research Highlights



Departments

Simulating Crystalline HMX Explosives

Livermore computer simulations exploring the effects of shock waves on crystalline HMX were featured on the cover of the May 14, 2015, issue of *Journal of Applied Physics*. The work, performed by staff scientist Ryan Austin and a team of Laboratory researchers, is part of a project to better understand the safety and performance of high explosives, such as HMX, which are used in the nuclear stockpile and by the Department of Defense.

The HMX crystals contain defects in the form of pores or bubbles. When shocked, the pores collapse and form "hot spots," which can produce small burning regions that propagate in a self-sustained manner. The interaction of burn and pressure fronts from many hot spots initiates the path toward detonation. Austin says, "From a mechanistic viewpoint, we still don't understand precisely how these burning reactions are initiated or how the transition to detonation occurs."

Austin employed state-of-the-art material models that put together most of the important physical processes. A significant finding of the simulations was prominent shear banding (melt cracking) around a collapsing pore—an effect derived from the strength response of the crystal. This behavior contrasts predictions from conventional strength models, which typically do not account for the anisotropic, and viscoplastic nature of crystal deformation. The simulations show reactions can be initiated within the shear bands (extended hot spots) on a nanosecond timescale, indicating that dynamic flow strength is an important consideration.

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Researchers Reveal New Electron Ring Formation

In recent laser wakefield acceleration experiments, a team of scientists from Livermore and the University of California, Los Angeles (UCLA), revealed new electron ring formations in addition to the typically observed beams. Using the ultrashort-pulse Callisto laser system (shown above) in the Laboratory's Jupiter Laser Facility, the team produced a plasma in a low-density gas-cell target. The research appeared in the July 31, 2015, issue of *Physical Review Letters*.

The interaction of the high-intensity laser with the gas created a relativistic plasma wave that then accelerated some of the electrons in the plasma to more than 100-megaelectronvolt energies. These electron beams are usually directed along the laser axis and have fairly low divergence. In certain cases, they were also accompanied by a second, off-axis beam that had a ring-like shape—a feature that has never been previously reported. UCLA collaborators performed computationally intensive three-dimensional calculations of the experimental conditions to determine the feature's origin. "The dynamics of the plasma wave are often calculated in simulations, but the small spatial scale and fast timescale of the wakefield process has made direct measurements of many effects difficult or impractical," says lead author Brad Pollock. "The discovery of new features allows us to confidently compare simulations with experiments." This work was partially funded by the Laboratory Directed Research and Development program.

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Laboratory Garners Three R&D 100 Awards

Three technologies developed by Livermore researchers and their collaborators received R&D 100 awards from *R&D Magazine* in its annual competition to honor top scientific and engineering technologies with commercial potential. This year's award winners are as follows:

- The Zero-RK software package speeds up simulations of chemical systems a thousandfold over methods traditionally used for internal combustion engine research.
- A three-dimensional printing instrument, called the Large-Area Projection Microstereolithography System, fabricates large products with highly detailed features.
- The High-Power Intelligent Laser Diode System is a compact, scalable laser system that achieves two-to-threefold improvement in peak output power and intensity over existing technology.

Contact: Richard A. Rankin (925) 423-9353 (rankin@llnl.gov).

First Stars Left a Unique Signature

Determining the chemical abundance pattern left by the earliest stars in the cosmos is important to understanding the evolution of the universe. An international team led by Livermore's Brian Bucher has made an important contribution to predicting the unique chemical signature left by early stars—which formed approximately 13.8 billion years ago—with the first direct measurement under stellar conditions of a nuclear reaction. This work appeared in the June 26, 2015, issue of *Physical Review Letters*. Bucher says, "Verifying the predicted composition of stellar ashes by comparing them to observational data is vital to our understanding the properties of the first stars and the formation of the first galaxies."

To accurately determine early stars' abundance signatures requires proper modeling of the stars and their nuclear reactions. One reaction that largely influences some key properties of the abundance pattern is the fusion of two carbon nuclei into a magnesium nucleus and one neutron. However, measuring stellar reaction rates in the laboratory is challenging because the likelihood

(continued on p. 24)

Commentary by Anantha Krishnan

Efforts Help Relaunch a Critical American Industry

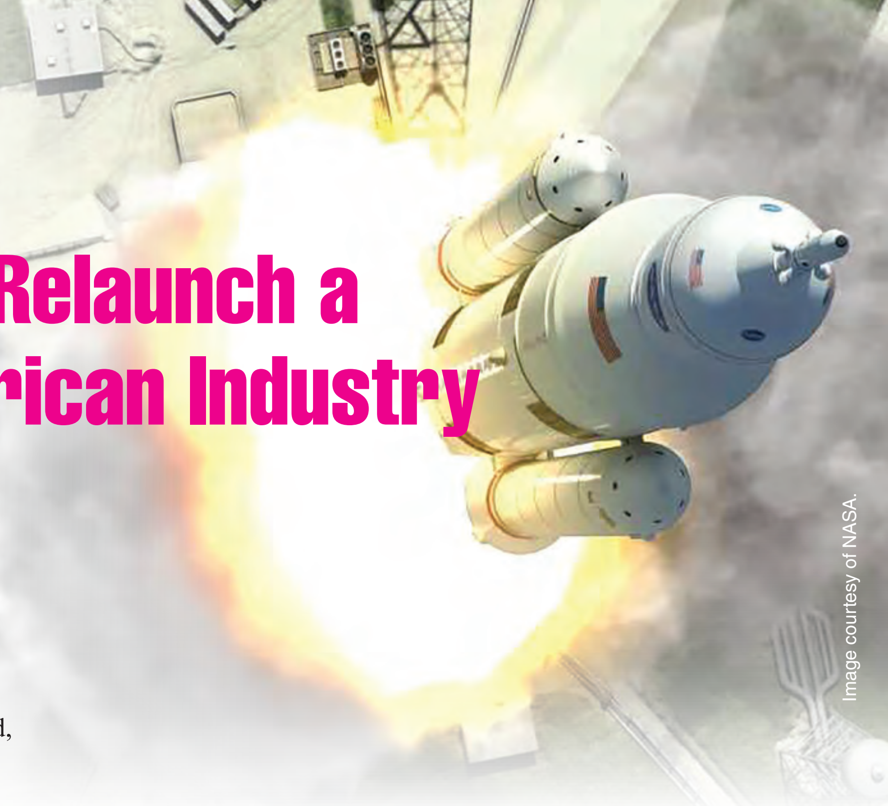


Image courtesy of NASA.

FOR more than a century, American scientists, engineers, technicians, and business leaders led the world in building the finest airplanes and, later, the most powerful rockets for national security and scientific exploration. More recently, U.S. government agencies have encouraged development of new technologies to drastically lower costs and increase innovations in rocket propulsion. In 2010, NASA's Space Shuttle was retired, and the past decade has witnessed the emergence of small and aggressive U.S. companies aiming to revolutionize the space-launch industry. These fledgling firms are creating new designs for liquid-fueled engines and reusable, manned launch vehicles that will significantly reduce the costs of putting people and payloads into space.

Laboratory scientists and engineers are demonstrating to many of these companies the power and utility of high-performance computing (HPC) in developing and assessing future technologies. Using computers as a virtual test bed has become a hallmark of Lawrence Livermore research. With HPC machines, scientists and engineers can evaluate new ideas, designs, and materials in silico before prototypes are built and tested. In this way, companies deliver new products into the marketplace more quickly and with less expense.

Lawrence Livermore efforts have now demonstrated the value of HPC in transforming the design and testing of new rocket engines and launch vehicles. Laboratory scientists and engineers have completed two space-technology ventures for the Defense Advanced Research Projects Agency (DARPA) and two ambitious small American companies. For the first project, the Livermore team simulated the performance of a novel liquid-propellant rocket engine intended for DARPA's Next-Generation Rocket program. The second effort used simulations to study the thermal and structural response of a design for DARPA's reusable launch vehicle called the XS-1.

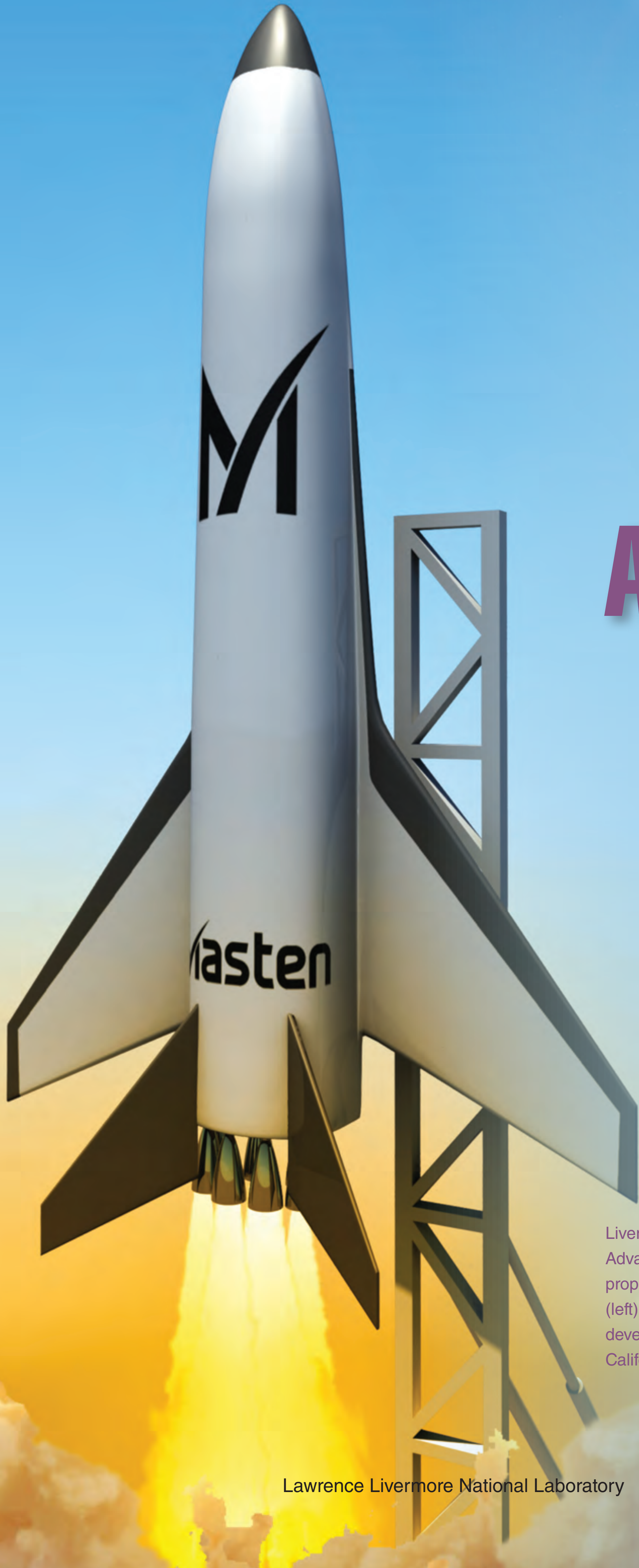
These endeavors have demonstrated Livermore's long-standing ability to quickly assemble teams comprising subject matter experts in a wide range of disciplines such as materials science; combustion chemistry and physics; flight aerodynamics, including thermal and structural stresses; and supercomputing simulation. The most advanced physics-based computational models were brought to bear on these projects to simulate the physical processes associated with liquid-fuel combustion and space-flight dynamics.

Using Livermore's Cab and Syrah supercomputers, engineers performed three-dimensional (3D) simulations using up to a 60-million-cell mesh on a 10-nanosecond and 10-nanometer scale to produce high-fidelity 3D simulations of a rocket engine in operation. While resolving short-lived temperature and pressure transients that influence the safety and efficiency of engine operation, the simulations provided some of the most detailed views ever of how oxidizer (liquid oxygen) interacts with the turbulent methane fuel. The Livermore team also performed simulations of the engine operating at up to 30,000 meters in altitude. For the launch-vehicle design, the team examined the flightworthiness of the system at various points along a simulated flight trajectory from liftoff to Mach 10 and back to vertical landing. In particular, the team, in collaboration with designers from the companies, studied stresses on the supports for the fuel tank.

Although HPC is an immensely powerful tool, researchers must ensure the physical models accurately represent the way materials behave when subjected to extreme environments. The Laboratory has a number of world-class facilities, such as the National Ignition Facility, High Explosives Applications Facility, and high-pressure laboratories, for conducting subscale experiments to validate advanced physical models.

Lawrence Livermore has a proven track record of helping American companies use HPC for designing and evaluating products to significantly reduce development time and cost. A pressing national need exists for a vigorous, domestic space-launch industry, and Laboratory scientists and engineers are leading the way in using HPC to ensure the industry's success and the effectiveness of the technologies it delivers.

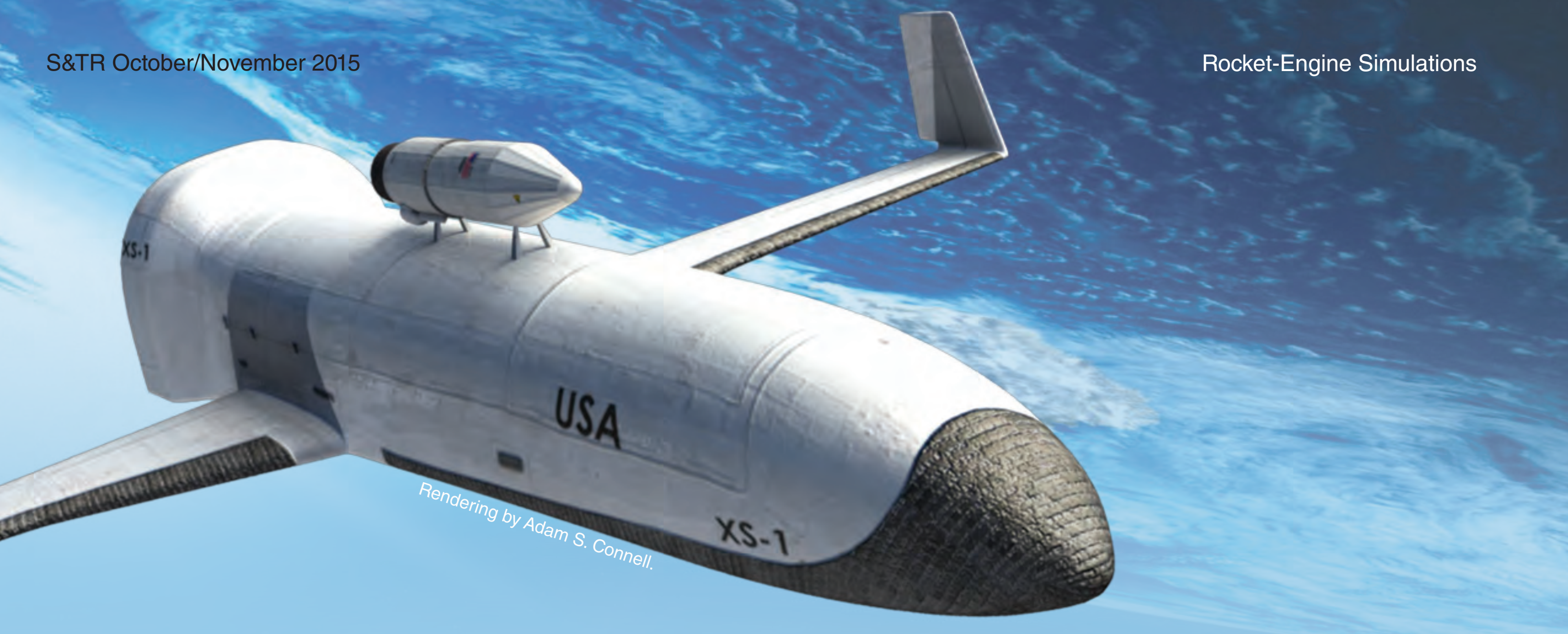
■ Anantha Krishnan is associate director for Engineering.



Advancing and the

Livermore researchers demonstrate the power of high-performance computing for developing aerospace technologies.

Livermore engineers are working with the Defense Advanced Research Projects Agency (DARPA) on a proposed medium-lift-capacity XS-1 space plane. (left) An artist's rendering illustrates an early design developed by Masten Space Systems of Mojave, California. (Figure courtesy of Masten Space Systems.)



Rendering by Adam S. Connell.

Next-Generation Rockets Engines that Power Them

FOR more than two decades, Lawrence Livermore researchers have pioneered the use of advanced simulation software and some of the world's most powerful supercomputers to virtually design, prototype, and test new components—and entire engineering systems—for national security missions. This approach represents a radical departure from legacy industry practices in which prototypes are typically designed, built, field-tested, broken, and then reworked, significantly increasing the time and expense of evaluating prototype architectures and materials.

In the past few years, Livermore engineers have exploited high-performance computing (HPC) to hone concept designs before prototypes are built and tested. In this way, advanced military systems that work flawlessly are delivered more quickly and at reduced cost. For example, the Livermore-developed BLU-129B low-collateral-damage munition, built for the Department of Defense (DOD), was produced in record time—the first prototype was produced in months rather than the typical years. (See *S&TR*, March 2013, pp. 4–9.) More recently, an interdisciplinary team of Livermore scientists and engineers used HPC to complete a shorter and significantly less expensive development and testing program for a hypersonic conventional warhead. The effort culminated in a sled test proving the design of the warhead and aeroshell and its carbon-based materials. (See *S&TR*, December 2014, pp. 4–11.)

In response to a national need for routine—and more affordable—access to space, Livermore researchers are developing new simulation tools, techniques, and expertise to make possible cost-effective rocket-engine and launch-vehicle designs for national security and scientific exploration. These new capabilities promise to significantly reduce the time, expense, and risk of realizing new space technologies. Livermore engineers and scientists are also creating and applying new additive-manufacturing methods to space technology applications that will enable faster and cheaper routine production of complex parts. (See the box on p. 11.)

Two Efforts for One Agency

In late 2014, a team of Livermore aerospace, mechanical, computational, materials, electronics, and systems engineers began work on two space-technology efforts for the Defense Advanced Research Projects Agency (DARPA). For the first project, researchers conducted a series of simulations directed at evaluating a novel liquid-propellant rocket engine (LRE) design intended for DARPA's Next-Generation Rocket (NGR) program. The simulations focused on the engine's injector performance, combustion characteristics, cooling system, thermal and structural characteristics, and altitude-compensating ability. "DARPA gave us 'seedling' funding to demonstrate our HPC and engineering capabilities for evaluating a new engine design," explains Bill Bruner, Livermore's NASA relationship manager.

The second effort used simulations for studying the thermal and structural response of a candidate launch-vehicle design for DARPA's proposed medium-lift-capacity XS-1 space plane. The XS-1 is envisioned as the first stage of a reusable launch vehicle that could fly 10 times in 10 days, exceed Mach 10 speeds at least once, and launch a payload of up to 2,267 kilograms into low-Earth orbit.

"We're showing DARPA managers we can use computation and modeling to decrease risk, expense, and development time," says aerospace engineer and computational physicist Greg Burton, who leads the Turbulence Analysis and Simulation Center (TASC) within Livermore's Computational Engineering Division. Most of the simulations for the two DARPA projects were conducted under the auspices of TASC.

Engineer Bob Addis, who helped manage Livermore's previous conventional warhead and sled test programs, notes the importance of HPC's cost-savings potential. He explains that in the past it has been more economical for NASA and DOD to purchase liquid-propellant rocket motors from Russia, rather than fund development of U.S.-made motors using legacy industry design practices and techniques. Addis and others are encouraged by the emergence of small, visionary U.S. firms with new ideas for putting payloads reliably and inexpensively into orbit, as well as by DARPA's interest in funding research to develop American-made next-generation launch vehicles and rocket engines.

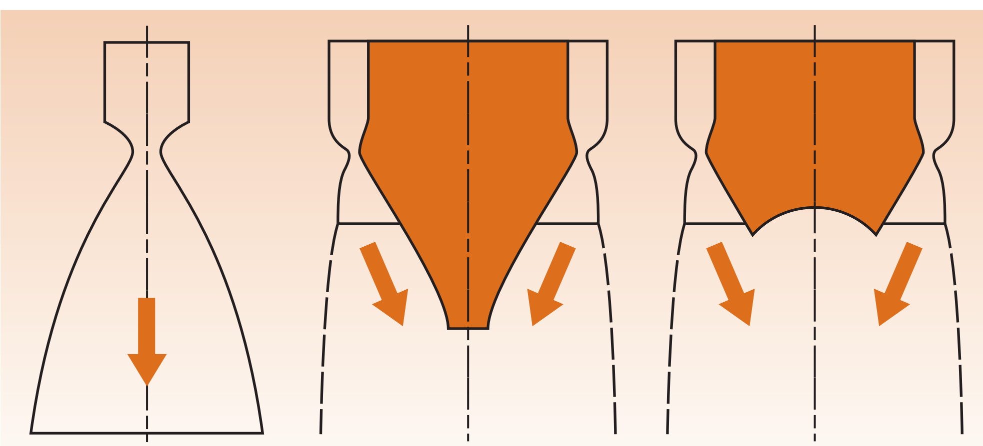
Computer-Testing a Rocket Engine

The first DARPA-sponsored effort was a partnership between Livermore and WASK Engineering of Cameron Park, California. Livermore engineers were tasked with creating and applying numerical tools to simulate WASK's design of an advanced LRE with an aerospike nozzle. The nozzle design features modular rocket thrust cells arranged in a ring around a novel zero-length central spike.

Measuring about 5 centimeters long and 2 centimeters across, each thrust cell can burn for 5 to 8 minutes and be reused at least 100 times. The cells feature an unusual fuel-injection system for mixing methane (fuel) with liquid oxygen (oxidizer). Each thrust cell resembles an inverted old-fashioned glass milk bottle, with the neck of the bottle representing the combustion chamber's throat. The combustion gases discharge to the nozzle (mouth of the bottle), where the gases are expanded, creating a powerful exhaust. Engineer Allen House, manager for both the aerospike LRE and launch-vehicle simulation projects, notes that WASK provided computer-aided design models of the thrust cell, as well as estimated values for combustion temperatures, pressures, and fuel flow rates.

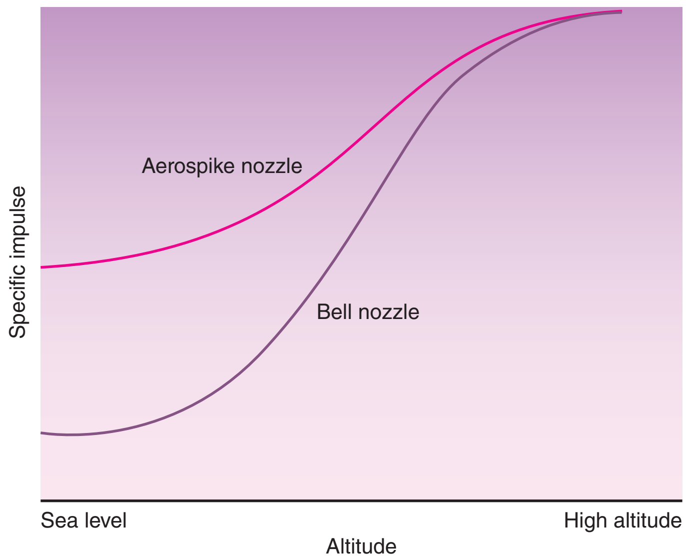
Aerospikes may be a more efficient alternative to the traditional bell nozzle, in which the exhaust emerges from the combustion chamber and expands against the fixed geometry of the nozzle wall, producing much of the engine's thrust. Bell nozzles operate at peak efficiency when the nozzle expands the exhaust to ambient atmospheric pressure at its exit. However, because ambient atmospheric pressure decreases as a rocket accelerates to orbit, bell-nozzle engines are most efficient at only one particular altitude. As a result, the rocket operates at less than peak efficiency through most of its boost to orbit, and thus must carry more fuel, thereby increasing its weight and decreasing both the altitudes it can reach and the weight of payload it can deliver.

Aerospike LREs, on the other hand, naturally compensate for changes in atmospheric pressure. Rather than expanding gases along a bell nozzle's fixed geometry, the aerospike both expands gases along the fixed wall of the central spike, which provides thrust to lift the vehicle, and to the open atmosphere on the other side. As the



(left) A traditional bell nozzle, (middle) an aerospike nozzle with 50-percent length, and (right) a zero-length aerospike nozzle all produce thrust as the exhaust gases press against the nozzle surface. The two aerospike configurations vent exhaust gases to the ambient environment on the outside of the spike but are able to maintain higher exhaust pressure at the spike surface than a traditional bell nozzle, thereby increasing the engine's thrust and efficiency.

spacecraft climbs to higher altitudes, the air pressure holding the exhaust against the open side naturally decreases, keeping higher pressure on the spike side. In this way, the exhaust geometry automatically adjusts to changes in pressure, and the engine more efficiently uses its available fuel over a wide range of altitudes.



A bell-nozzle engine's peak efficiency is achieved when the nozzle expands the exhaust at its exit to the ambient atmospheric pressure at a particular altitude, and achieves lower efficiency both above and below that altitude. This notional graph shows the efficiency (specific impulse) of an aerospike design versus a bell nozzle optimized for a high altitude. The aerospike achieves more thrust compared to a bell nozzle at most altitudes of operation.

Inside Aerospike Engines

Simulating any LRE is a multiphysics problem that includes transport and mixing of oxidizer and fuel at challenging pressures, densities, and temperatures; complex combustion chemistry; and convective and radiative thermal transport. Coupling and studying these phenomena requires prodigious computational resources. Fortunately, Burton's team had at its disposal the Laboratory's massively parallel supercomputers that use tens of thousands of processors in tandem. These machines were used to run established Livermore codes, commercial codes, and two computational fluid dynamics (CFD) codes that were initially developed at Stanford University's Center for Turbulence Research. Together, these codes describe the flow and mixing of methane and liquid oxygen; reactions and concentrations of the chemical compounds involved in combustion; efficacy of the engine-cooling system; temperature distribution and resultant thermal stresses important for analyzing the structural strength of the thrust cells; and structural and thermal loads during takeoff, flight, and landing.

The two Stanford turbulent mixing and combustion codes, CharlesX and JOE, were originally developed as part of the Department of Energy's (DOE's) Predictive Science Academic Alliance Program to simulate combustion in a high-Mach-number scramjet engine—an air-breathing jet engine in which combustion occurs in a supersonic stream of gas. The codes were substantially modified and enhanced by the Livermore engineering team so they could accurately simulate a functioning LRE like the WASK aerospike design.

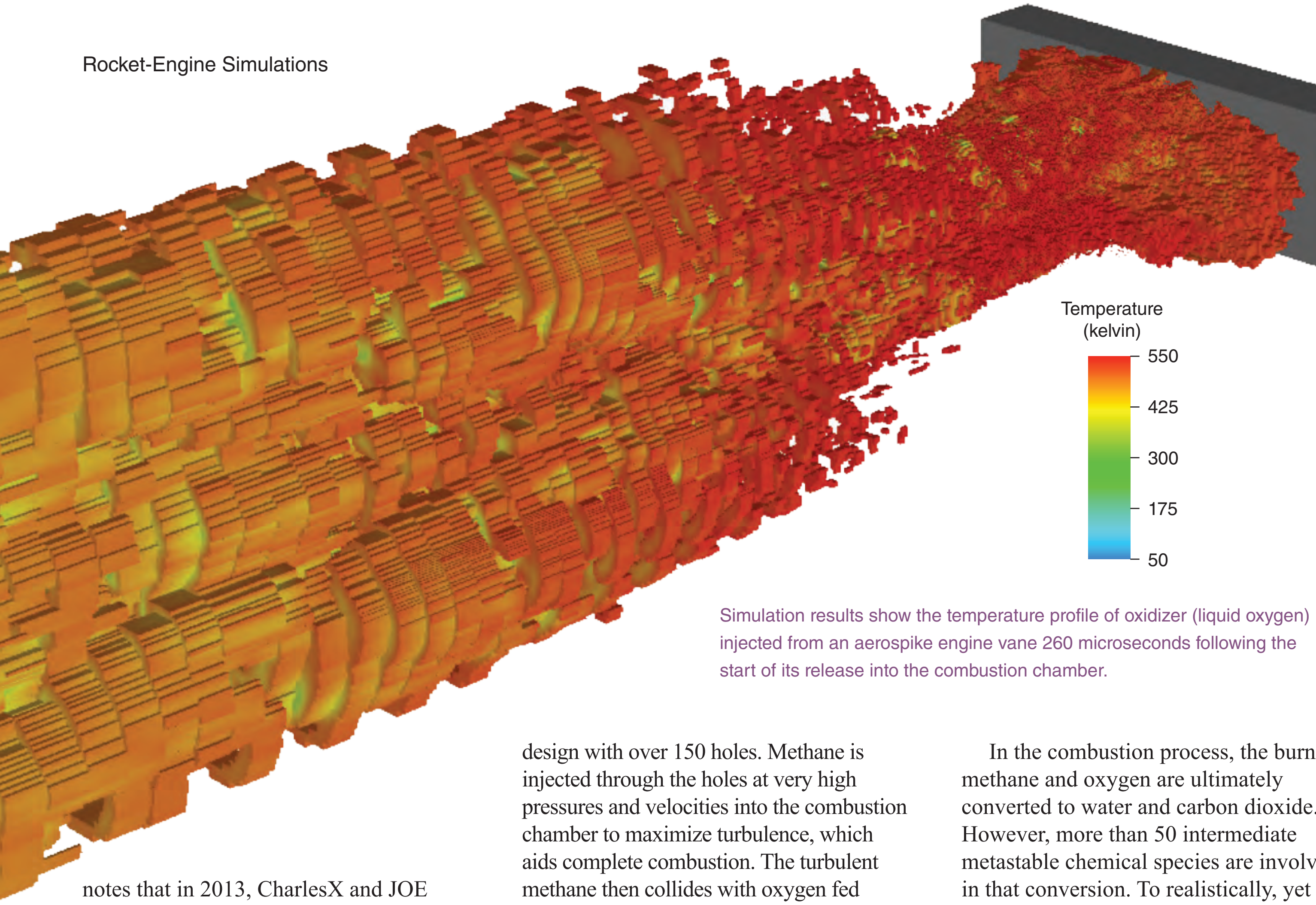
Sister Codes CharlesX and JOE

CharlesX is a state-of-the-art turbulent combustion large-eddy simulation (LES) code for resolving the transient events that occur during turbulent mixing of fuel and oxidizer and their subsequent combustion. The simulations detail important features such as heating and other high-stress transients, which can prematurely age or damage engine walls or potentially cause catastrophic failure of the engine and the launch vehicle. By contrast, sister code JOE is a Reynolds-Averaged Navier Stokes (RANS) simulation code, which resolves only steady-state features.

Simulations using both codes were conducted on Livermore's Cab and Syrah supercomputers. Team members Matt McNenly, Nick Killingsworth, Ryan Vignes, and summer student Elyce Bayat conducted three-dimensional (3D) simulations on two meshes, a moderately resolved 9-million-cell mesh, often used for RANS simulations, and a much finer 60-million-cell mesh for LES runs. The 9-million-cell mesh permitted millimeter-to-nearly-micrometer spatial resolution, thereby allowing simulations to proceed faster than with finer meshes. "It helped us quickly examine coarse features within the system with reasonable accuracy," says Burton. The 60-million-cell mesh resolved certain transient flow and combustion features on the 10-nanosecond and 10-nanometer scale.

The simulations used as many as 4,096 cores (central processing units) over 200 hours of processing time, to successfully isolate features of the transport, mixing, and combustion of the oxidizer and fuel in a thrust cell. The result was one of the highest fidelity 3D simulations of an operating rocket engine ever performed. Burton says the simulations provided insight into how the WASK injector design affects performance, as well as the temperatures and pressures generated during combustion that may affect engine efficiency and stability.

Implementing such fine meshes and large numbers of processors is unprecedented for LRE simulations. Says Bruner, "HPC to traditional rocket designers typically means using one-hundredth the number of cores that we do. Such simulations can provide some design insight but do not allow the level of risk reduction we can achieve with many times additional computing power." Burton

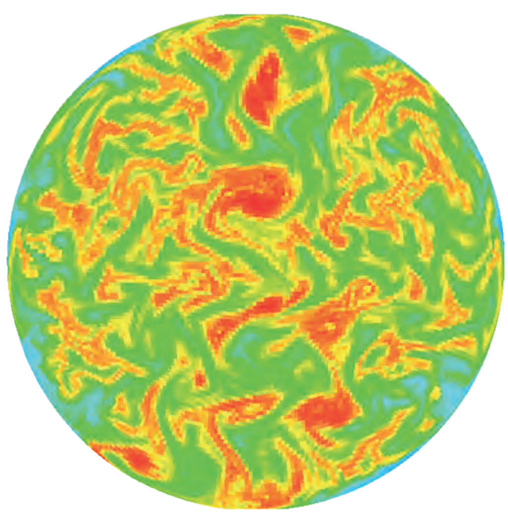


Simulation results show the temperature profile of oxidizer (liquid oxygen) injected from an aerospike engine vane 260 microseconds following the start of its release into the combustion chamber.

notes that in 2013, CharlesX and JOE were successfully run on other projects at high efficiency when scaled up to 1.5 million cores on Livermore's Sequoia supercomputer. Bruner and Burton look forward to future work where simulations of this magnitude may significantly improve accuracy of results.

A Turbulent Process

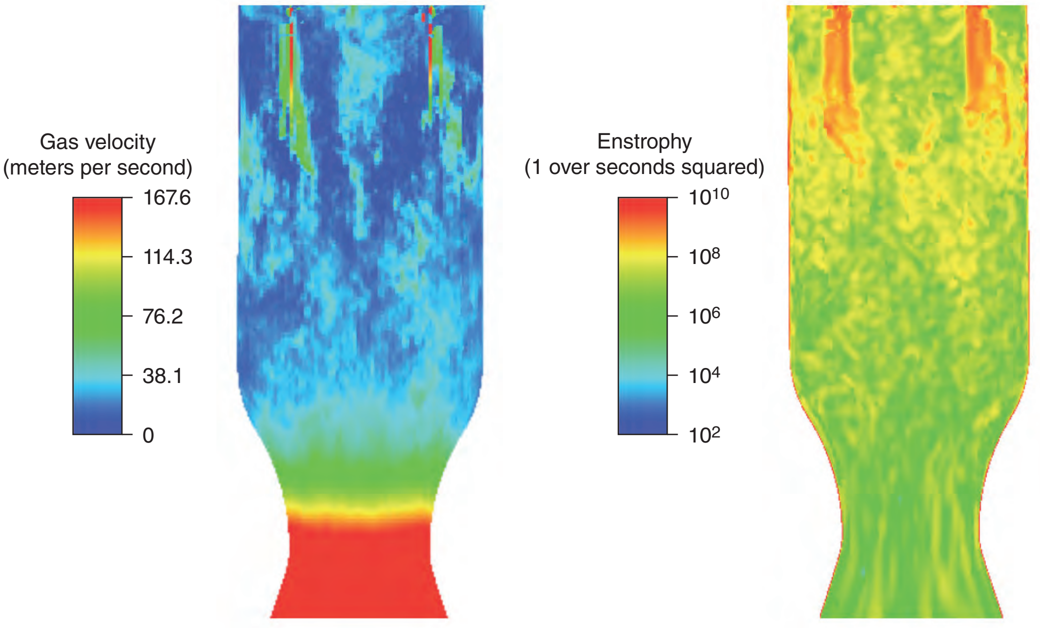
The team first examined how the system mixes fuel and oxidizer at the head of the combustion chamber. The researchers used a computational mesh that almost exactly reproduced the geometry of the injection system, which features a "showerhead" design with over 150 holes. Methane is injected through the holes at very high pressures and velocities into the combustion chamber to maximize turbulence, which aids complete combustion. The turbulent methane then collides with oxygen fed into the chamber through a series of vanes. Burton's team also performed both RANS and LES simulations of a single vane to better understand how the oxidizer interacts with the turbulent methane. The simulations confirmed previous experimental studies that showed the dominant mixing mechanisms. The results were then used to initialize simulations of the combustion chamber.



Using CharlesX software and a 9-million-cell mesh, researchers analyzed temperature fields within an aerospike thrust-cell combustion chamber. This cross section of the chamber shows real-time combustion details on a submicrosecond timescale as well as the location of flame fronts (shown in orange).

In the combustion process, the burning methane and oxygen are ultimately converted to water and carbon dioxide. However, more than 50 intermediate metastable chemical species are involved in that conversion. To realistically, yet efficiently, simulate this complicated process, the Livermore team combined CharlesX and JOE with Stanford's Flamelet Progress Variable (FPV) model. The FPV model uses a pre-tabulated chemistry database to relate traditional measures of a combustion system, such as species concentration and heat release, to other variables calculated by the simulation. A combustion–reaction model developed by McNenly was combined with FPV to incorporate these chemical intermediaries and provide a more complete picture of combustion. "Chemicals react and produce intermediaries when they burn," explains McNenly. "This approach is an effective way to capture the most important aspects of the combustion reaction."

By tracking the mixing of fuel and oxidizer and the complex chemical reactions involved in combustion, the simulations show how efficiently and stably the engine can generate the



Researchers applied a 9-million-cell mesh to simulate the operation of a thrust-cell combustion chamber. Longitudinal cross sections of the chamber show (left) the gas exhaust velocity and (right) the enstrophy—a measurement that approximately denotes the intensity of the mixing process.

hot gases needed to power a launch vehicle. LES combustion studies yielded instantaneous "snapshot" views of mixing and flame dynamics throughout the engine from the injector and then combustion chamber, to downstream of the throat by the nozzle. The simulations reveal random, tiny, and highly transient phenomena when burning stops (called blowouts), often followed by reignition. Such phenomena can create temperature spikes that make combustion unstable and capable of engine damage. McNenly notes that the simulations indicate that the faster the mix, the more complete the combustion.

Keeping It Cool

An integral part of the aerospike's proper functioning is its cooling system. "The combustion chamber must be continually cooled or it will burn up," explains Livermore engineer Pete Fitsos. Combustion temperatures can reach 3,500 kelvin, but the cooling system must reduce those to 700 kelvin at the thrust cells' outer walls.

The combustion chamber is composed of a high-conductivity copper-alloy liner surrounded by a structural inconel (high-performance alloy) barrel. To maintain uniform cooling and avoid damaging thermal stresses, cryogenic methane flows through a network of 2-millimeter-wide channels that wrap around the copper liner. The warmed methane is then injected into the combustion chamber.

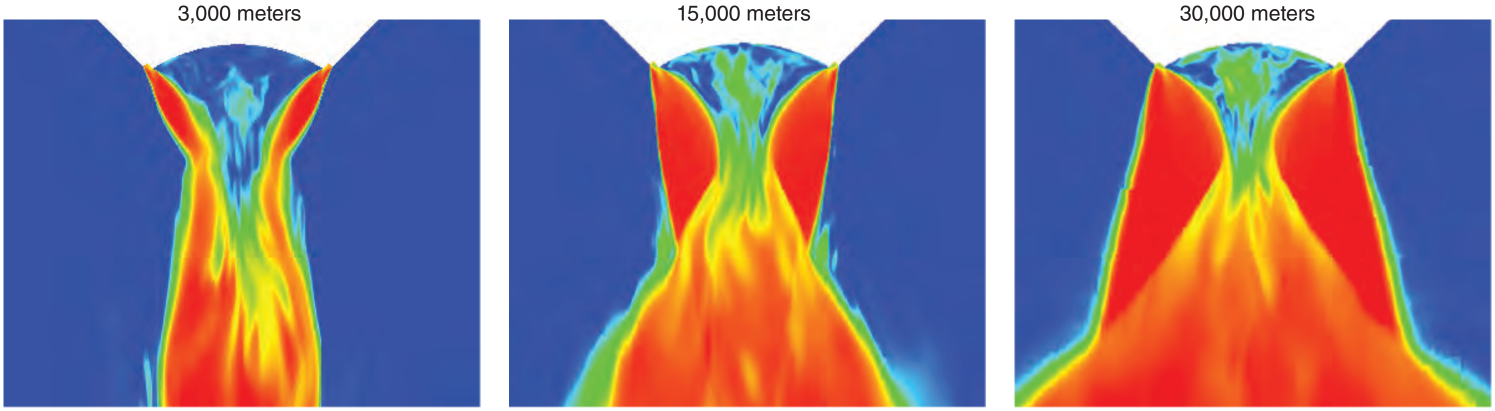
To model the interplay between the cooling liquid and the combustion chamber, Fitsos began with a temperature–pressure profile generated by the CFD simulations. He then used commercial codes to obtain a temperature distribution describing how heat is transferred to an individual cooling channel. The result was a 3D view of the locations and magnitudes of the stresses generated as the copper liner expands and pushes against the inconel frame. The temperature distribution was imported into a model that calculated the overall structural loads on the thrust cell from combustion-generated temperature gradients and pressures.

A reusable rocket engine undergoes punishingly large temperature and pressure swings during its use. Calculating thermal stresses is important because they can be the limiting factor in the lifetime of the engine. Fitsos says data generated by the simulations can indicate areas that might become overstressed during normal operation, which could result in engine and launch-vehicle failure. Follow-up simulations can then determine the effectiveness of any proposed design modifications. Fitsos says, "We have shown that with our computational resources and the right codes, we can do more detailed work than was previously possible."

Simulating External Aerospike Flow

Near the end of the project, Burton agreed to conduct the first-ever 3D LES study of the time-varying turbulent flow from an external aerospike exhaust plume. Starting with the thrust-cell exhaust conditions indicated by the earlier internal combustion simulations, he ran three simulations at altitudes of 3,000; 15,000; and 30,000 meters using the full 3D aerospike geometry. The same grid size was used for each simulation, with the highest resolution aimed at capturing the intense turbulent dynamics generated by the thrust cells' exhaust on the aerospike engine's surfaces. The simulations ran on 2,048 cores of Cab for 250 hours each.

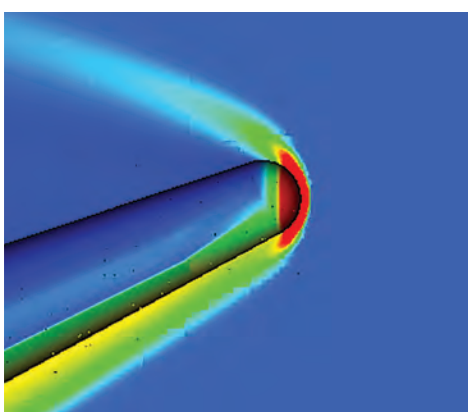
The resulting exhaust flow fields were used to estimate overall engine performance and to evaluate the altitude-compensating behavior of the aerospike engine design. To complete these new



Three simulations show the exhaust flows of an aerospike engine at altitudes of 3,000; 15,000; and 30,000 meters. The simulations reveal that in contrast to conventional rocket-engine designs, the aerospike design compensates for altitude differences.

simulations on schedule and within budget, the team introduced certain approximations that led to specific impulse (a measure of rocket-engine efficiency) estimates nearly 8.5 percent smaller than prior analytical estimates. Burton expects that in future work configured without the approximations, results will range much closer to analytical estimates.

Importantly, "We calculated that the engine does in fact compensate for altitude differences, and in the same amount predicted by analytical studies," says Burton. "We can thus say with some confidence that at least this particular aerospike design exceeds the performance of conventional bell engines."



Livermore simulations have shown the temperature distribution on the nose of a hypersonic vehicle, such as the XS-1, as it re-enters the atmosphere. Colors denote relative temperatures.

Assessing Structural Soundness

The aerospike engine could one day fly on a launch vehicle like DARPA's proposed XS-1 hypersonic vehicle. Livermore engineers provided DARPA aerodynamic–thermal–structural analysis on a proposed vertical-takeoff and vertical-landing design concept for the XS-1 developed by Masten Space Systems of Mojave, California. The team combined aerodynamic and thermal stresses generated by Burton's CFD simulations with structural modeling using NIKE3D, a code developed at Livermore. The engineers assessed the mechanical integrity of the Masten design at various points along a simulated flight trajectory from liftoff to Mach 10 and back to vertical landing.

Over several months, Burton and engineer Will Elmer iterated with Masten design engineers to evaluate the structural integrity of the company's evolving XS-1 design. "We aided Masten in selecting structural designs that satisfied DARPA's flight requirements," says Burton. The effort included analyzing critical components such as the vehicle's liquid fuel tank. In one instance, the simulations showed the superiority of a design refinement to structural components supporting the fuel tank.

"Masten needs to be confident that their launch-vehicle design is controllable under all flight conditions," says Elmer. One focus of the study was the performance of the plane's four flaps (or fins) that provide important aerodynamic stability. Elmer explains,"We analyzed the drag and lift on the flaps to ensure no oscillation of the vehicle would occur in flight." The team also examined the integrity of the flaps' connections to the vehicle.

RANS and LES codes analyzed thermal and pressure stresses resulting from the extreme changes in temperature and outside aerodynamic pressures as the launch vehicle fulfilled its mission to place a payload into low-Earth orbit and return to the launch pad. The engineers provided snapshots of the structural and thermal loads on the vehicle at points along its simulated flight trajectory. "Through this work, we can show companies how to catch problems early and save money," says Elmer.

Ready to Partner

"With the past successful DOD programs and the most recent work for DARPA, we have demonstrated what's possible in a short timeframe with HPC," says Bruner. "We can model combustion and flight processes with a level of fidelity that can significantly shorten expensive development cycles, while increasing confidence in the design." As a result, Bruner envisions engaging to a much greater degree with the space flight community to offer Livermore's computational and additive-manufacturing services. However, he

Additively Manufactured Rocket Parts

An efficient technology design cycle requires rapid and cost-effective prototyping. The complex shapes of many rocket components makes additive manufacturing a faster and cheaper tool for providing prototype—as well as flight-ready—parts, when compared to conventional fabrication techniques. For example, the myriad tiny channels of an aerospike thrust-cell cooling system pose significant manufacturing challenges.

Over the last few years, Livermore engineers and materials scientists have demonstrated additive-manufacturing capabilities for producing parts with unique properties pertaining to density, strength, extreme geometry, and surface finish. These capabilities could produce liquid propellant rocket engines (LREs) for components that are stronger, more efficient, lighter, and heat resistant than those available from traditional manufacturing techniques. Such components could improve the efficiency of the engine, allowing larger payloads to be launched with reduced risk into low-Earth orbit.

In 2013, Livermore engineers demonstrated the potential of additive manufacturing when they worked with a small-firm rocket designer. The engineers successfully "printed" a full-scale prototype LRE containing convoluted cooling channels that could not be made by conventional manufacturing techniques. Livermore materials engineer Stephen Burke supervised the effort. Burke started with a computer-aided design file provided by the customer, which was converted to an industry-standard file appropriate for three-dimensional printing. The motor was made from powdered stainless steel particles measuring 30 micrometers in diameter. The particles were fused together using Livermore's laser-welding machine, which laser-welds one layer of powdered particles at a time. The machine ran unattended over 8 days, 24 hours per day, producing thousands of layers, each 25-to-30-micrometers thick.

Burke says that using conventional manufacturing methods, the rocket motor would have had to been made in several pieces and then welded together. "We built one complete piece about 26 centimeters long and 10 centimeters in diameter," he says. "We can build parts now that used to be impossible to manufacture."

Livermore engineers manufactured this rocket motor with an additive-manufacturing process using stainless steel particles measuring 30 micrometers in diameter.

emphasizes that any partnership must be the "right fit," working with a company that understands the enormous potential of HPC.

Burton and his team have been spreading the word about Livermore's space-technology presence. They presented their findings at an important Joint Army–Navy–NASA–Air Force propulsion conference in Tennessee last June. Burton has also made presentations to DARPA and DOE. He says, "We now have a family of computational tools to use on sufficiently powerful computers and the experience implementing them, allowing us to study for the first time the performance of rocket engines and launch vehicles to unprecedented levels of detail."

House adds, "We have the HPC systems, codes, expertise, and additive-manufacturing tools to jump-start the rocket industry in a new direction." Addis predicts the adoption of HPC will spark cost-effective rocket engines and advanced launch vehicles that could eventually reduce launch costs from the current $10,000 per pound to about $100 per pound. He says, "We're on the brink of a rocket-engine revolution."

—Arnie Heller

Key Words: additive manufacturing, aerospike, Cab supercomputer, CharlesX, computational fluid dynamics (CFD), Defense Advanced Research Projects Agency (DARPA), Department of Defense (DOD), Flamelet Progress Variable (FPV), high-performance computing (HPC), JOE, large-eddy simulation (LES), liquid-propellant rocket engine (LRE), Next-Generation Rocket (NGR) program, Predictive Science Academic Alliance Program, Reynolds-Averaged Navier Stokes (RANS), Sequoia supercomputer, Stanford University Center for Turbulence Research (CTR), Syrah supercomputer, Turbulence Analysis and Simulation Center (TASC), XS-1 launch vehicle.

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Image courtesy of NASA

Turning an X-Ray Eye on Universes, LARGE and SMALL

ANSWERS to many scientific mysteries lie in realms invisible to the human eye. Clues to some of the most fundamental questions in astronomy, cosmology, and nuclear science lurk in sections of the electromagnetic spectrum outside the small slice of wavelengths one can see. To better understand questions of scientific and national importance, the Laboratory has ventured into research involving a wide electromagnetic spectrum, from the longest radio waves to the shortest gamma rays.

As a part of this mission, scientists and engineers at Lawrence Livermore have created and nurtured a world-recognized expertise in the art and science of developing x-ray optics. Beginning in the 1970s, x-ray optics were designed and installed in high-energy-density physics diagnostics for early laser systems such as Shiva and Nova. Two decades later, the Laboratory honed its optics skill by participating in the Extreme Ultraviolet Lithography (EUVL) program—a unique government–semiconductor industry collaboration formed to explore using extreme ultraviolet wavelengths for fabricating next-generation computer chips. (See *S&TR*, November 1999, pp. 4–9.) Livermore's Michael Pivovaroff, an associate division leader for physics in the Physical and Life Sciences Directorate, notes, "The Laboratory's contribution to the quarter-billion-dollar EUVL project involved a large multidisciplinary team of scientists and engineers with special knowledge in x-ray optics, photon–material interactions, deposition technology, and materials science. Since that time, we have been stewards of this expertise and the accompanying capabilities, including magnetron sputtering, metrology, and modeling the properties of x-ray optical systems."

The Laboratory has been called upon throughout the last two-plus decades to develop x-ray optics for a variety of projects and programs, including high-energy-density physics experiments at the National Ignition Facility, astrophysics research, and synchrotron science. More recently, Livermore x-ray optics prowess has played a role in creating special x-ray telescopes designed to detect the dark matter of the universe and in developing instruments to assay the makeup of spent nuclear fuel.

Tuning Reflectivity

Although x rays are subject to the same phenomena as visible light—reflection, refraction, reflection—designing optical structures to effect those properties is challenging. As Chris Walton, a materials scientist in Livermore's Condensed Matter and Materials Division, explains, "For x rays to completely reflect, they must graze the surface of an optic, striking at a small, glancing incidence angle. Furthermore, the higher the energy of the x ray, the trickier it becomes to design an optic for reflectivity." Photons of high-energy x rays are strongly absorbed by matter such as air or the lens material and are thus hard to guide and direct.

Two common designs that use grazing incidence mirrors to collect and focus x rays are Kirkpatrick-Baez (KB) and Wolter optics. KB optics are two grazing incidence reflective mirrors that focus x rays to an appropriate detector or film. Although KB optics have few parts to assemble, they have less light-gathering area, which makes it difficult to image a weak source. The Wolter family of designs, which includes telescopes, has substrates with more complexity that allow concentric shells of x-ray mirrors to be "nested" inside one another to achieve large light-gathering areas.

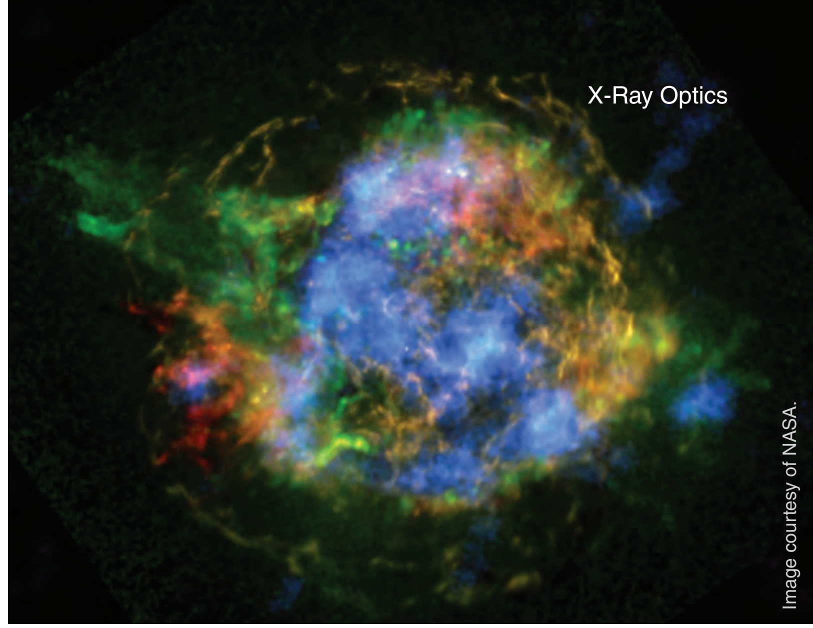
Multilayered structures are common in both types of optics. Developing multilayer-coated x-ray optics—including relay mirrors, telescopes, microscopes, and filters—has become a Livermore specialty. For these systems, precise, multilayer coatings of alternating materials are deposited upon super-smooth substrates. "These systems can consist of hundreds to thousands of bilayer pairs," Walton says. "We vary the types of materials used, their thicknesses, and other properties to carefully tune the reflectivity for specific applications."

The Mystery of Dark Matter

One of the big unknowns in cosmology involves the composition of the universe. Only about five percent of its composition can be observed directly—the rest is "darkness." Dark energy (roughly 68 percent) has no mass and is accelerating the expansion of the universe. Dark matter (about 27 percent) has mass but does not interact easily. Its presence is deduced by its gravitational effect on visible matter.

Several theories exist on what kinds of particles constitute dark matter. A strong contender is the axion, a hypothetical subatomic particle that is very light and electrically neutral. If they exist, axions could be detected when they are converted to photons in the presence of strong magnetic or electric fields. This phenomenon could, in theory, create axions in the Sun and is the basis for most strategies to detect the elusive particle.

CERN's Axion Solar Telescope (CAST) uses a prototype dipole magnet from the facility's Large Hadron Collider as the basis for a solar-axion detector. The 9-tesla magnetic field acts as a catalyst to transform axions into x rays. CAST has been collecting data since 2003, and Livermore joined the international experiment in 2005. Last year, a Laboratory-led team that included researchers from Columbia University and the Technical University of Denmark (DTU) Space National Space Institute built a new x-ray telescope for CAST based on the Wolter telescope design. This telescope is designed to focus axions that



Lawrence Livermore has a long history of developing advanced x-ray optics for viewing portions of the electromagnetic spectrum typically invisible to the human eye. Such optics are part of NASA's Nuclear Spectroscopic Telescope Array (NuSTAR), which images hard x rays ranging in energies from 3 to 79 kiloelectronvolts (keV). This image of the supernova remnant Cassiopeia A shows high-energy x-ray data (blue) captured by NuSTAR. Lower energy x rays previously recorded from the Chandra X-ray Observatory are shown in red, yellow, and green.

had been converted into x rays and increase the signal-to-noise ratio by a factor of approximately 100, while simultaneously allowing an accurate measurement of the background signal. The entire system was operational for the first time in the summer of 2015.

Livermore is now turning an x-ray eye to the International Axion Observatory (IAXO), a proposed system for CERN that aims to acheive a signal-to-noise ratio 100,000 times better than CAST. This substantial improvement is made possible by building dedicated

A transmission electron microscope image shows a cross section of an optic made with alternating thin-film layers of zirconium (dark bands) and carbon (light bands) on a silica (silicon dioxide) substrate. The zirconium is dark because it more strongly absorbs and scatters electrons as well as x rays, making it useful in x-ray mirrors.

The CERN Axion Solar Telescope (CAST) features a test magnet (blue structure) from CERN's Large Hadron Collider. The magnet is supported by the green "cradle" that also holds cooling and electrical equipment. The yellow structure and railroad tracks allow the apparatus to follow the Sun as it changes position relative to Earth.

subsystems including a large magnet, optimized x-ray optics, and low-background detectors. The heart of IAXO will be a superconducting magnet with eight large bores that maximize the axion-to-photon conversion area. Each of the eight magnet bores will be equipped with Livermore-designed x-ray-focusing optics based on a Wolter telescope design. The proposed optics consist of nested, highly reflective mirrors that will reflect x-ray photons at shallow grazing incident angles, directing the photons to sensitive x-ray detectors.

IAXO optics are envisioned to be similar to those installed on NASA's Nuclear Spectroscopic Telescope Array (NuSTAR)—an x-ray astrophysics satellite with two focusing telescopes that operate in the 3-to-79-kiloelectronvolt (keV) energy band. NuSTAR's optics, also developed in part by Lawrence Livermore, consist of thousands of thermally formed glass substrates deposited with complex multilayer coatings to enhance the reflectivity above 10 keV. Todd Decker, a Livermore engineer who played a key role in building NuSTAR's x-ray telescope, says, "We learned more about making telescopes from our involvement with NuSTAR, and we have many good ideas on how to improve substrates as a result."

Focusing X Rays for Nonproliferation

The capability to nondestructively examine and measure the content of specific isotopes of interest is critical to nuclear safeguards and nonproliferation. Livermore's Marie-Anne Descalle is the principal investigator for a project funded by the Laboratory Directed Research and Development (LDRD) Program to create mirrors that measure hard x rays for nuclear security. She explains, "The ability to detect hard x-ray or soft gamma-ray emissions (photons ranging up to several hundred kiloelectronvolts) from special nuclear material plays an important role in a number of national security applications." One such application is the nuclear safeguards required for treaty obligations.

Hard x-ray optics offer one path to dramatically improve detection performance. These optics effectively collect the photons emitted from relatively weak sources, such as uranium-235 or plutonium-239, and filter out nuisance sources that obscure a significant spectral signature. She notes, "With just a bare detector, the spectral lines of interest in a spent fuel rod are overwhelmed by the high count rates emitted by cesium-137 and other isotopes. In essence, the lines of interest are simply drowned by the noise."

The project had many challenges to overcome. "We didn't know for certain whether multilayers would work well above the 100-kiloelectronvolt threshold, and we needed to detect photons ranging up to several hundred kiloelectronvolts," says Descalle. She and the LDRD team built on efforts first funded by the Department of Energy's Office of Defense Nuclear Nonproliferation Research and Development to characterize multilayer systems and create a new class of optics and conduct tests with flat mirrors. The LDRD funding allowed the team, which included researchers from Livermore's Physical and Life Sciences and Engineering Directorates, as well as collaborators from DTU and the European Synchrotron Radiation Facility (ESRF), to study photon interactions with multilayers in the hard x-ray band and produce robust, inexpensive, and high-accuracy mirror substrates. They tested their optics at ESRF, one of the only x-ray light sources in the world with sufficiently bright beams to investigate photon energies as high as 750 keV, and measured x rays of energies above 500 keV.

Livermore researchers, including (left to right) Regina Soufli, Marie-Anne Descalle, and postdoctoral researcher Nicolai Brejnholt, have demonstrated that multilayer coatings deposited on super-polished substrates operate efficiently as reflective optics at photon energies up to 650 keV. Brejnholt is shown here holding a highly polished square x-ray mirror, which due to an optical illusion appears pyramidal.

The researchers have also benchmarked a simulation code to predict the performance of optimized coatings for various applications and conducted an experiment at Livermore's Jupiter Laser Facility, successfully demonstrating the technique in high-energy-density plasmas and expanding applications for hard x-ray optics. The experiment used flat mirror substrates. Future experiments will use curved x-ray mirrors, which provide better information by filtering out more of the undesirable hard x-ray lines. Pivovaroff notes, "For hard x-ray mirrors, alignment becomes more difficult because shallower grazing angles are needed at higher energies. New types of substrates will help us overcome some of these challenges."

Descalle's team has been working on several cost-effective techniques for creating substrates, including chemical treatment of plastic and new methods to slump (heat) glass. Preliminary results on the plastic show some promise, but Descalle and Decker are particularly interested in a type of extremely thin glass for creating a substrate that is highly flexible. Descalle says, "We need to understand how the flexibility of the glass may affect the coating process, the material's shape, thermal transport, and other properties. Our team has the expertise to solve the challenging issues related to this work."

The Laboratory's 40-year foray into x-ray optics research and development has been highly successful. "We support the Laboratory's core missions and basic science efforts, from helping to solve some of cosmology's more vexing questions to providing details about special nuclear materials," says Pivovaroff. "In maintaining our optics expertise from the time of the EUVL program, Livermore experts can create multilayer materials with different properties and deposit them on curved optics for concentrating images, or on flat optics for relaying x-ray photons or filtering spectral signals. This work is an institutional strength that stretches across the breadth of the Physical and Life Sciences and Engineering Directorates. By making the invisible visible, we are helping deliver solutions to scientific questions of national importance."

—Ann Parker

Key Words: astronomy, astrophysics, axions, CERN Axion Solar Telescope (CAST), dark matter, Extreme Ultraviolet Lithography (EUVL) program, gamma rays, high-energy-density research, International Axion Observatory (IAXO), Kirkpatrick-Baez (KB) optic, Laboratory Directed Research and Development (LDRD), magnetic field, multilayers, NASA Nuclear Spectroscopic Telescope Array (NuSTAR), nonproliferation, special nuclear materials, Wolter telescope, x-ray optics.

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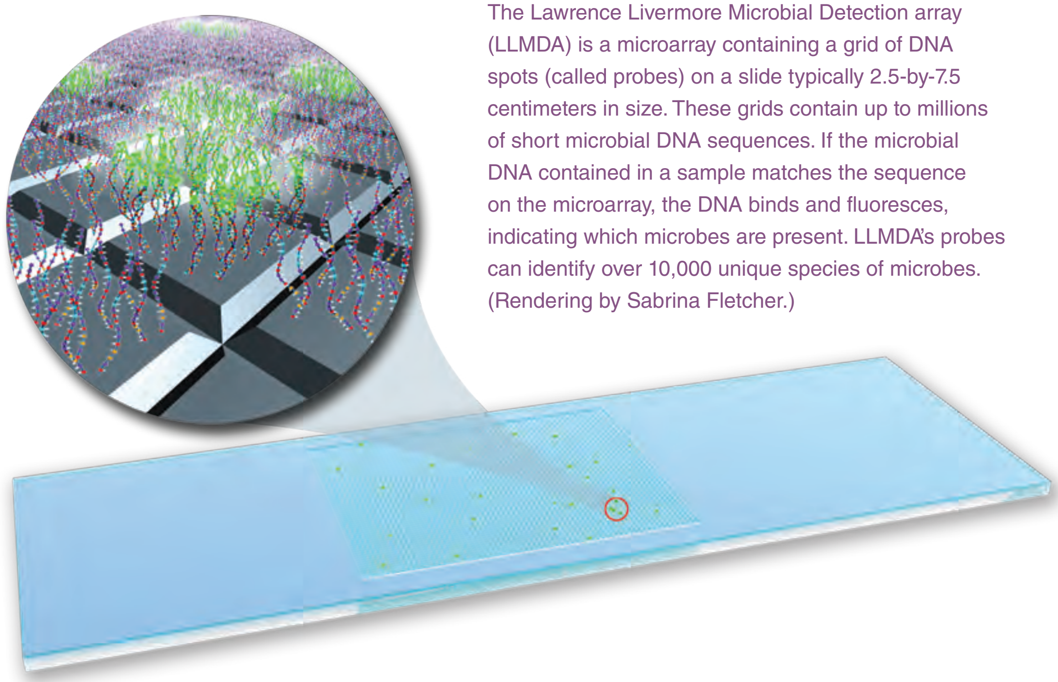
Two-Part Microbial Detection Enhances Bioidentification



The Lawrence Livermore Microbial Detection array (LLMDA) is a microarray containing a grid of DNA spots (called probes) on a slide typically 2.5-by-7.5 centimeters in size. These grids contain up to millions of short microbial DNA sequences. If the microbial DNA contained in a sample matches the sequence on the microarray, the DNA binds and fluoresces, indicating which microbes are present. LLMDA's probes can identify over 10,000 unique species of microbes. (Rendering by Sabrina Fletcher.)

A military medical team responding to an infantry soldier with extensive wounds must quickly deduce the most effective way to treat the victim. Typically, clinicians determine a wound-care approach based upon general intuition and experience. This approach must include considerations such as the optimal time to close the wound, how healing will be affected if the wound is closed immediately, which antibiotics to administer, and how other factors—including what bacteria may be in the wound—could help or hinder the patient's overall recovery.

New microbial detection technologies may help clinicians make more informed treatment decisions specific to a patient's needs. Laboratory researchers have recently demonstrated an approach that uses the Lawrence Livermore Microbial Detection Array (LLMDA) and the Livermore Metagenomic Analysis Toolkit (LMAT) for identifying and quantifying microbes to improve patient care. LLMDA offers a quick, cost-effective initial screening of a sample from a patient's wound. LMAT, on the other hand, provides more thorough examination of microbes by analyzing the exact order of chemical bases that form their DNA, called sequences, to identify pathogens and their genetic attributes.

"A perfect world of pathogen surveillance and diagnostics is analogous to a wheel and a spoke," explains LMAT principal investigator Jonathan Allen. "LLMDA is the wheel's hub—a high throughput screening tool that processes and categorizes the majority of information. The spokes are LMAT's sequencing methods, which provide deeper analysis of a sample, for identifying any initially undetected data or for gathering additional details." Used together, these two technologies are serving as the basis to transform biodefense efforts and improve medical treatments.

One Way or Another

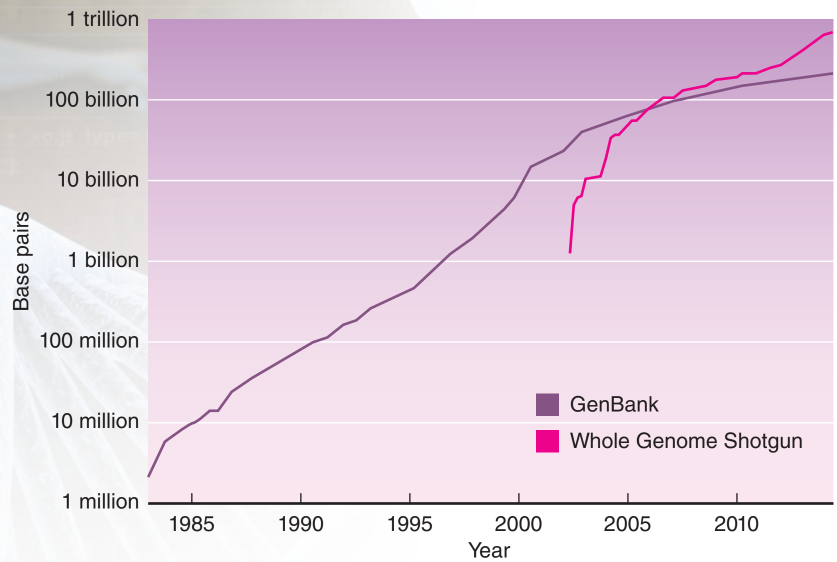
LLMDA is a microarray containing a grid of DNA spots on a 2.5-by-7.5-centimeter slide. (See *S&TR* April/May 2013, pp. 4–11). These grids contain hundreds of thousands to millions of short microbial DNA sequences, which are the complements of genetic markers found in microbes. If the microbial DNA contained in a fluid genetic sample matches the sequence on the microarray, the DNA binds and fluoresces, indicating which microbes are present. Traditional pathogen identification methods require up to several days to analyze a sample, but LLMDA boasts a 24-hour processing time. LLMDA can identify more than 10,000 unique species of microbes. However, the system can only detect previously sequenced microbes whose DNA complement is included on the array.

In contrast, LMAT delivers specific genetic information for microbes and identifies any that have been previously sequenced. LMAT's open-source software searches through genetic data catalogued in public repositories to more specifically identify organisms. In fact, a major accomplishment of LMAT is its ability to compile genetic variation into a searchable, scalable, and comprehensive database—a feat never before accomplished.

The vast amount of genetic information contained in microbial whole-genome repositories, currently totaling 115 gigabases and growing, posed significant challenges for the LMAT team. "Many bioinformatics problems are memory constrained because too much data is available," says computer scientist Maya Gokhale, who researches solutions to big-data problems in many fields, including metagenomics. These challenges will continue to grow as gene sequencing becomes easier, cheaper, and faster to execute, and as available genomic data increases exponentially. To overcome these memory and data storage problems, the LMAT team turned to innovations in supercomputing hardware and software.

Big Data, Big Memory

Gokhale and her team addressed LMAT's big-data issue by applying cutting-edge storage and access methods. "Our development approach to LMAT's metagenomic analysis and classification was centered upon anticipating the very large



As genome-sequencing processes become easier to execute, the amount of genome sequence data steadily increases with time. This graph shows sequenced genome data measured in base pairs over time, from two genome databases. The data influx poses a need for scalable software such as the Livermore Metagenomic Analysis Toolkit (LMAT), which enables users to identify pathogens including diseases, bacteria, viruses, fungi, and other organisms.

memory that would be required," says Gokhale. The flash drive, a type of nonvolatile random-access memory (NVRAM), provides a supplemental memory resource for retaining data even when the processor's power is off. Spreading database storage across NVRAM uses less main memory, called dynamic random access memory (DRAM). Unlike conventional storage structures that use disk memory, LMAT's use of both flash and main memories increases processing speeds.

LMAT was run on Livermore's Catalyst cluster to test the data storage and analysis approach. Catalyst is a first-of-its-kind architecture whose design was influenced by Gokhale and her team's memory storage research. The system is equipped with an impressive amount of both main and flash memories, which makes it ideally suited for solving big-data problems. LMAT was copied into the flash memory of each of Catalyst's 324 nodes. Individual nodes contain 800 gigabytes of flash memory alone.

However, the team's use of both main and flash memory made it difficult to retrieve data. "Traditionally, to access data, it has to be stored in DRAM," explains Gokhale. To retrieve needed data from both memories, Gokhale's team created a clever caching algorithm that transparently fetches a DNA sequence from NVRAM and moves it into DRAM, and from DRAM into the central processing unit.

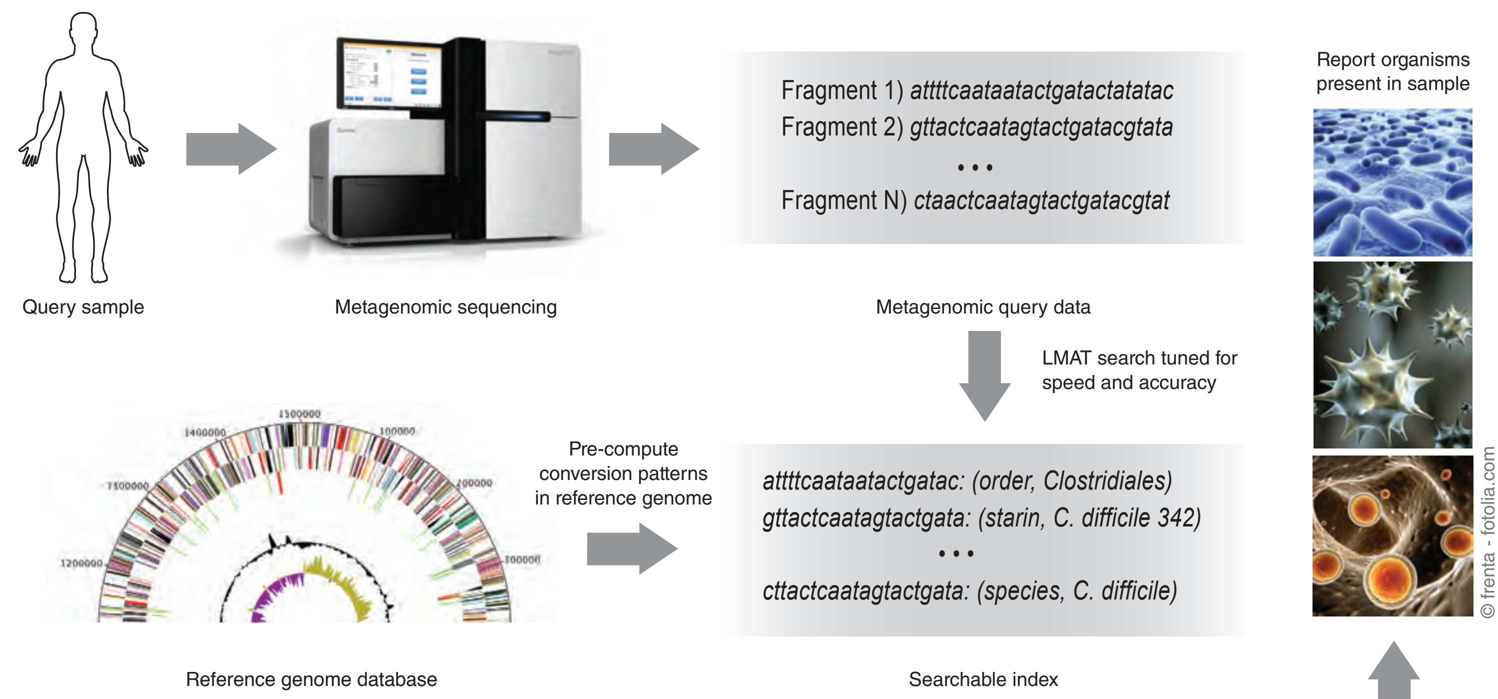
The caching system analyzes small sequences of genomic data called k-mers—continuous genetic sequences of length *k*. The team compiled all previously sequenced microbial genomes and broke them into short, contiguous sequences, where the k-mer length was 20 base pairs. Each k-mer was tagged by its source genome and marked according to its taxonomic level, which defines groups of biological organisms on the basis of shared characteristics. When LMAT identifies a k-mer, the database also indicates possible related organisms according to its taxonomic label. Looking at all the matching k-mers for a query sequence, Allen created an algorithm to select the taxonomic classification, which best reflects the taxonomic classification of the individual matching k-mers.

Furthermore, the team developed a method for faster retrieval of frequently fetched items. Index data is split into two components: data held in main memory and data held in flash memory. As an example, the first 10 base pairs of the k-mer may be cached in main memory if they have been searched for previously. K-mers similar to the sample in main memory then point to additional k-mers stored in flash memory that share the sample's first 10 base pairs. This complete process reduces trips to the flash drive, improving data retrieval time.

Catalyst has demonstrated LMAT's capabilities and is a proven asset for the approach. However, computers of its caliber are uncommon to other laboratories and universities, which limits LMAT's potential user base. "Our strength is our weakness," explains Allen. "Our index requires computing resources with a certain sophistication that is not readily accessible to many users." Thus, Allen is working to build an Amazon "instance," a virtual server containing LMAT, on Amazon's Elastic Compute Cloud for running applications via Amazon Web Services. Amazon account holders could download the instance and run LMAT remotely. "Our ultimate goal is to increase access to the technology," says Allen. "Those who do not have Livermore's computing resources or expertise should still be able to leverage LMAT's sequencing analysis."

The Treatment Two-Step

When used in conjunction, LLMDA and LMAT can help clinicians make more informed treatment decisions by identifying



Using LMAT, nucleic acids extracted from a query sample undergo sequencing to recover short genetic fragments. Fragments are searched against an index to identify organisms present.

specific bacteria in a wound that could affect the healing process. Laboratory researchers tested the dual approach on wound samples from 44 patients. LLMDA was used to assess 124 samples from combat wounds that had different healing outcomes. A subset of samples was then sequenced and processed by LMAT. In several cases, LMAT detected organisms LLMDA had not. The system could also potentially identify microbes that harbor antibiotic-resistant genes—a testament to its sensitivity of sequencing and LMAT's proficiency for detecting organisms in minute amounts.

"The combination of both technologies offers an effective workflow," explains microbiologist Nicholas Be. The team identified all present microbes—bacteria, viruses, and fungi—in the healed versus unhealed samples to compare microbial influence on the overall outcome. Results indicated that the presence of certain bacteria in the wound was associated with either positive or failed healing. Some types of bacteria, such as *Escherichia coli* and *Salmonella*, commonly found in the human gastrointestinal tract, were more frequently observed in wounds that healed successfully. This result defies traditional assumptions that all bacteria are malignant and should be eliminated and supports the notion that more specific microbial information better guides wound-treatment decisions.

"Thanks to these Livermore-developed technologies," says Be, "our team determined that it's insufficient to merely look at a wound for microbe presence or wound cleanliness and base treatment on that assessment." These findings could lead to improved wound-treatment processes in the clinic as well as in the field, as metagenomics researchers are working to make microbial detection technologies portable.

LLMDA and LMAT are products of an impressive combination of unique algorithms, microtechnology, and multidisciplinary collaboration. These innovative technologies have already aided in disease detection for the commercial swine industry, surveillance for emerging viral diseases, and pathogen identification in ancient DNA, such as that from the time of the 14th century Black Death. In the future, LLMDA and LMAT will continue to drive pathogen-detection efforts for human medicine and bioterrorism.

—Lanie L. Rivera

Key words: algorithm, bacteria, big data, biodefense, bioterrorism, caching, Catalyst supercomputer, disease, dynamic random access memory (DRAM), fungi, gene, genome, k-mer, Lawrence Livermore Microbial Detection Array (LLMDA), Livermore Metagenomics Analysis Toolkit (LMAT), medicine, metagenomic, microbe, microarray, nonvolatile random-access memory (NVRAM), pathogen, sequencing, surveillance, virus, wound.

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Thermite Research Heats Up

ENERGETIC materials—explosives, propellants, and pyrotechnics—are substances that store and release large amounts of chemical energy. They are made by either physically mixing solid oxidizers and fuels to produce a composite energetic material, such as gunpowder, or by creating a molecule that contains both oxidizing and fuel components, such as TNT. The total energy released during the chemical reaction—the energy density of the material—can be much greater for composites than for single-molecule energetic materials, but the rate at which composites release energy is much slower (that is, the power is lower). (See *S&TR*, October 2000, pp. 19–21.)

Laboratory scientists have begun to remedy this trade-off between energy density and power. "With composite materials, the particles have to diffuse much further to mix, which slows the reaction," explains Livermore materials chemist Alex Gash. "Although composites will never be like explosives, we can make them react faster by making their particles smaller." Twenty years ago, scientists discovered that shrinking fuel and oxidizer particle size from the micrometer to the nanometer scale boosts composite reactivity by at least three orders of magnitude. Consequently, efforts to improve reactivity have focused on refining particle size and other methods for decreasing the distance particles have to travel.

Livermore mechanical engineer Kyle Sullivan studies thermites, a type of pyrotechnic composite made from a metal fuel and metal oxide that rapidly burns up when ignited. Because of the focused, intense heat thermites provide, they have traditionally been used for applications such as metal joining and cutting. Sullivan, Gash, and fellow Livermore researcher Joshua Kuntz have examined the effect of fuel size on reactivity by initiating thermite reactions in clear acrylic burn tubes and recording the resulting flame propagation with a high-speed camera. They found that below three micrometers in diameter, decreasing particle size has rapidly diminishing returns.

The results redirected the team's focus. Rather than concentrating on how to optimally mix ingredients into a loose powder, Sullivan and colleagues, with funding from the Laboratory Directed Research and Development Program, have been exploring the feasibility of tailoring reactivity by controlling the mesoscale architecture. Three-dimensional (3D) thermite structures may be able to boost reaction control and reproducibility to enable new applications for these materials.

A Tiered Solution

Building a thermite architecture that achieves the desired behavior for a given application requires an in-depth understanding of reaction phenomena and the key variables governing them. "Part of the challenge is that we are dealing with nanoparticles. Much of their behavior is unknown compared to that of bulk materials," notes Sullivan. Further, when thermites ignite, many processes happen almost simultaneously—particles melt and decompose, and heat and gases are released—making it difficult to unravel details about the path from reactants to products with sufficient spatial or temporal resolution. The researchers' strategy has been to approach the problem in a tiered way, by looking at thermite behavior at multiple length and timescales.

At the nanometer and nanosecond scales, Sullivan's team has applied in situ dynamic transmission electron microscopy (DTEM), a Livermore-developed technology, to capture material response to rapid heating. In a DTEM experiment, a short laser pulse rapidly heats a small region of a specimen, initiating material transformations. A camera captures images or diffraction patterns of the dynamic process with as little as 10 nanoseconds of exposure time and as fine as 10-nanometer spatial resolution. (See *S&TR*, October/November 2013, pp. 8–9; September 2013, pp. 4–11.) For these experiments, the researchers heated and probed nanometer-scale aluminum particles, a common thermite fuel, to isolate fuel behavior during a thermite reaction.

When exposed to air, aluminum particles form an oxide shell. For nanometer-scale particles, the shell makes up a substantial fraction of the particles' volume and can have a significant effect on their behavior. For instance, aluminum's melting temperature is well below the melting point of the aluminum oxide shell, leading some researchers to theorize that as the thermite is ignited and the material undergoes rapid heating, the aluminum will melt and expand while the shell remains solid, causing the particles to burst. However, during the Livermore experiments, the heated particles did not break up. Rather, they quickly—within tens of nanoseconds—melted and coalesced into larger particles.

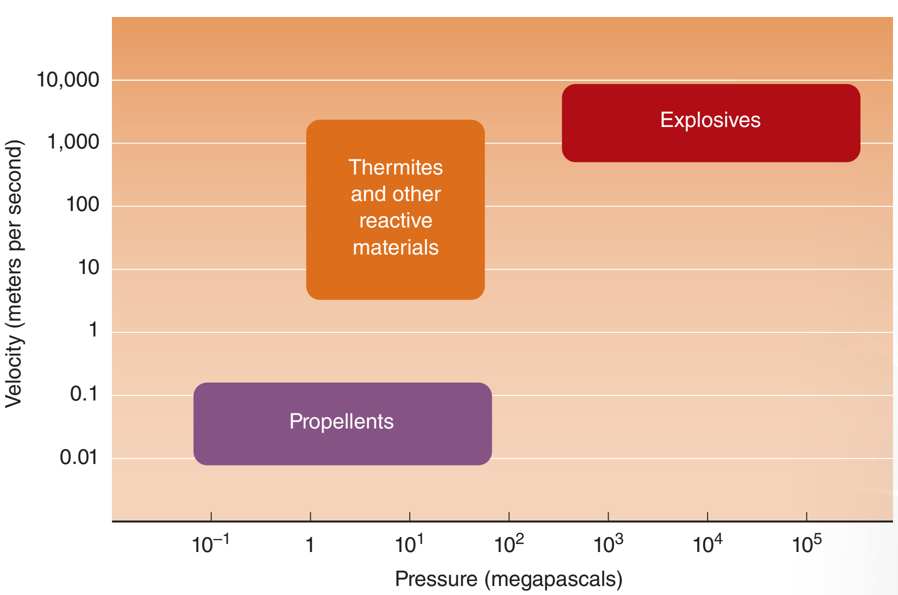
Gash notes, "DTEM debunked many speculative theories on what happens during a reaction." If thermite fuel particles are merging before they combust, this behavior could help explain the plateauing burn speeds witnessed in the experiments on particle size, as coalescence reduces the surface area available for reactions with the oxidizer. The results support the idea that future reactivity enhancements will likely come from methods other than reductions in particle size.

Role of Gases and Particles

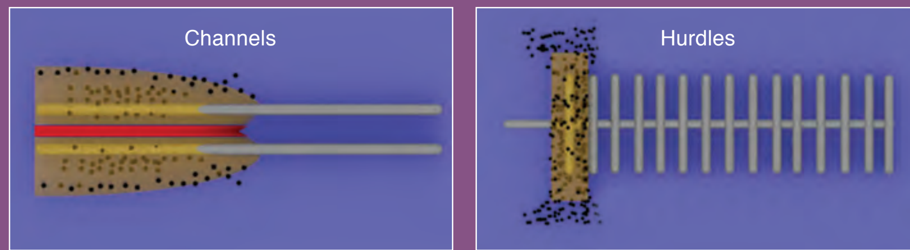
To better understand behavior at the micrometer and millisecond scales, the Laboratory researchers explored burn propagation on two-dimensional thermite tracks of various patterns and thicknesses. First, they created aluminum–copper oxide nanoparticle films using electrophoretic deposition (EPD), an additive manufacturing (AM) technique in which particles can be deposited onto a conductive electrode with precisely controlled thickness and mass (see *S&TR*, April/May 2015, pp. 19–22). The researchers then ignited the thermites and captured the reactions with high-speed imaging. Thick films (155 micrometers) were found to react nearly 10 times faster than thin films (26 micrometers), suggesting that feature size plays a role in reactivity. The team attributed this behavior to the increased thickness permitting more intermediate gases to be trapped, which builds pressure internally and promotes foward energy transport. In studying EPD as a method for incorporating themites into microelectromechanical or microenergetic devices, the team noticed that flames could travel down crooked paths, around corners, and across gaps, suggesting the reaction is driven forward by a complex interplay between gases and hot particles.

Experiments at the mesoscale have thus far focused on how neighboring 3D thermite structures interact with one another. The researchers, in conjunction with Livermore engineer Chris Spadaccini's AM team, used direct ink writing (see *S&TR*, March 2012, pp. 14–20) to build 0.5-millimeter-high substrates of silver, which were subsequently coated with an EPD-applied aluminum–copper oxide film. The silver structures were printed in two orientations and with different separation distances. Some sets of structures, called channels, were deposited parallel to the thermite burn path, while others, called hurdles, were positioned perpendicularly. Channel and hurdle flame propagation behaviors were compared with one another and with thermites deposited on a flat surface for a baseline comparison.

Both distance and directionality affected the reaction speed. Below a certain spacing in channels, the researchers observed an increase in speed—up to two to three times the baseline speed. By contrast, speeds gradually increased as the hurdles were spaced further apart, from values below the baseline to those similar to the peaks reached by the channel reactions. Through high-speed imaging, the team observed that in the channel arrangement,



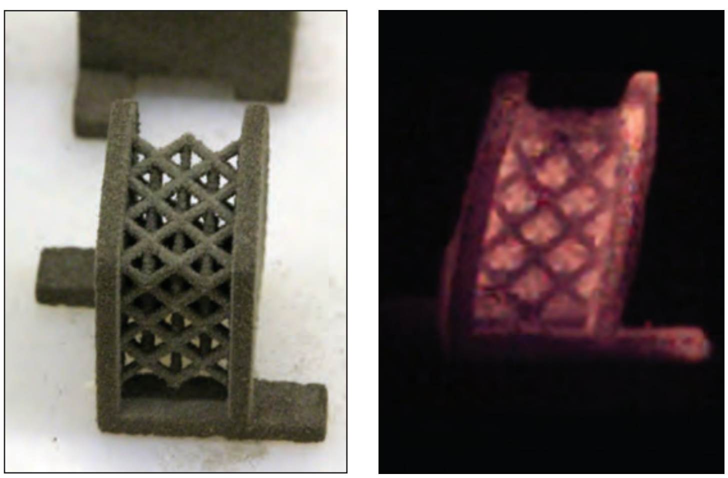
Thermites occupy a useful middle ground between slow-burning propellants and fast-acting explosives. Energy dense, relatively cheap, environmentally benign, and tunable, thermites are attractive for a number of applications that require an on-demand release of chemical energy. (Shown here are approximate velocity and pressure ranges for various energetic materials.)



Three-dimensional (3D) thermite test structures illustrate how architectural features can be used to better understand and tailor thermite behavior. (left) Parallel channels experience overlapping reaction waves that accelerate reaction speed. (right) Perpendicular hurdles, depending on their spacing, can either help or hinder the reaction by either misdirecting reaction waves or propelling hot particles forward.

gas release by the ignited thermite expands perpendicular to the direction of the reaction propagation. If the channels are close enough, the expansions can physically overlap and promote energy transport by propelling hot gases forward.

Hurdles behave differently. If the reacting material encounters the next hurdle before the reaction and gas expansion is fully developed, the expansion is interrupted, the reaction impeded, and the material pushed sideways. However, with the right separation, hurdles can enhance the reaction by “throwing” molten particles from hurdle to hurdle. “The hurdles play a game of toss and catch,” says Sullivan. “If the barriers are far enough apart, the particles can be transported a long way and ignite downstream material.” Not only did the mesoscale experiments help researchers understand gas and particle behavior, but they also successfully demonstrated that 3D architectural features such as spacing and orientation can be used to tailor thermite reactions.



Livermore researchers are designing, building, and testing 3D reactive structures, including both thermite and intermetallic formulations. An example skin-lattice design, produced by engineer Robert Reeves, is shown (left) before and (right) during a reaction. Ongoing work is examining the trade-off between material reactivity and strength and investigating how materials such as this can be used as structural components in energetic systems.

More Control, Greater Utility

Livermore researchers are currently using various techniques to print 3D structures of reactive materials. AM methods and 3D architectures are offering a new level of control over thermite reactions. Previous results are driving architecture designs, for example, by informing the feature size and orientation of the members within a part. The precision placement of energetic material in complex architectures can provide a user with additional ways to control the reactivity or explore new applications. For instance, these parts could replace inert structural components in a system. These materials could then contribute to the energy release, and their performance could be tailored through their design. Other applications involve microelectromechanical components, complex heat sources for thermal batteries, or 3D metal-joining tools.

Lawrence Livermore’s decades of research in energetic materials, its unique characterization tools such as DTEM, and its robust 3D printing and materials assembly infrastructure have together enabled an effective new approach to boosting thermite reactivity and reproducibility. The team is optimistic about the method’s broader utility. “Instead of developing new molecules and formulations,” notes Sullivan, “architectural control provides us an opportunity to further exploit the energetic materials we already have.”

—Rose Hansen

Key Words: additive manufacturing (AM), direct ink writing, dynamic transmission electron microscopy (DTEM), electrophoretic deposition (EPD), energetic material, nanoparticle, pyrotechnic, thermite.

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Patents and Awards

In this section, we list recent patents issued to and awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory. For the full text of a patent, enter the seven-digit number in the search box at the U.S. Patent and Trademark Office's website (http://www.uspto.gov).

Patents

Diffractive Optical Elements for Transformation of Modes in Lasers
Arun K. Sridharan, Paul H. Pax, John E. Heebner, Derrek R. Drachenberg, James P. Armstrong, Jay W. Dawson
U.S. Patent 9,124,066 B2
September 1, 2015

Modular Microfluidic System for Biological Sample Preparation
Klint A. Rose, Raymond P. Mariella, Jr., Christopher G. Bailey, Kevin Dean Ness
U.S. Patent 9,144,799 B2
September 29, 2015

Full-Wave Receiver Architecture for the Homodyne Motion Sensor
Peter C. Haugen, Gregory E. Dallum, Patrick A. Welsh, Carlos E. Romero
U.S. Patent 9,146,311 B2
September 29, 2015

Directly Driven Source of Multi-Gigahertz, Sub-Picosecond Optical Pulses
Michael J. Messerly, Jay W. Dawson, Christopher P. J. Barty, David J. Gibson, Matthew A. Prantil, Eric Cormier
U.S. Patent 9,166,355 B2
October 20, 2015

Awards

Laboratory geochemist **Annie Kersting**, who serves as the director of Livermore's Glenn T. Seaborg Institute, has been selected to receive the **2016 American Chemical Society's Francis P. Garvan–John M. Olin Medal**. The medal recognizes outstanding scientific achievement, leadership, and service to chemistry by women, and is a national award open to all chemists who are U.S. citizens. Kersting is well known for her work in actinide environmental chemistry. She was among the first scientists to show that insoluble radionuclides, like plutonium, could travel several kilometers in the subsurface environment as suspended, nanometer-sized colloidal particles. This work changed how scientists think about migration of insoluble actinides. Most of her current research at the Seaborg Institute focuses on better understanding what processes occur at the nanoscale—at the mineral–water surface that control the behavior of actinides in the subsurface. The goal is to predict and ultimately constrain the migration of these contaminants in the environment.

Anne Harrington, the National Nuclear Security Administration (NNSA) deputy administrator for Defense Nuclear Nonproliferation, presented the **NNSA Excellence Medal** to **Leon Berzins** for the successful **Source Physics Experiment 4 Prime (SPE4) campaign** at the Nevada National Security Site. The experiment, designed to provide a better understanding of seismo-acoustic propagation, is important to worldwide nuclear monitoring. In his role as manager of the SPE4 campaign, Berzins led the research team in redesigning experimental tools and methods, conducting safety reviews, coordinating efforts with Los Alamos National Laboratory, and fielding the experiment, which was successfully executed on May 21, 2015.

Lawrence Livermore scientist **Nir Goldman** recently received a $500,000 **NASA grant** to continue astrobiology research that aims to discover whether comets and other large astrophysical bodies delivered the complex prebiotic materials, amino acids, and peptides necessary for promoting life on Earth. Goldman's early research found that the impact of icy comets (containing simple molecules such as water, ammonia, methanol, and carbon dioxide) crashing into Earth billions of years ago could have produced a variety of small prebiotic or life-building compounds, including amino acids. The NASA grant will fund quantum simulation studies to understand aqueous mixtures of preformed amino acids under impact conditions. Goldman's efforts will extend his previous work by looking at whether extreme pressures and temperatures from impact could induce the formation of more intricate chemical structures such as peptide chains or simple proteins.

SPIE, the international society for optics and photonics, recently named Livermore researchers **Nerine Cherepy** and **Michael Pivovaroff** among 171 new **senior members**. SPIE senior members are honored for their professional experience, active involvement with the optics community and SPIE, and significant performance that sets them apart from their peers. Cherepy is being recognized for her "achievements in discovery and development of new scintillator materials and detectors," and is currently involved in creating new scintillator materials and instrumentation for gamma-ray spectroscopy and radiographic imaging. Pivovaroff is an associate division leader for physics, who leads the Applied Physics section, which investigates the nature of dark energy and dark matter, explores the dynamics of ultrafast photon–matter interactions, and performs observations to better understand the composition and distribution of planets and neutron stars. He is being recognized for his "achievements in design, fabrication, and use of reflective x-ray optics."

(*continued from p. 2*)

of producing a reaction is rare. The team successfully measured the carbon-fusion reaction at stellar energies using a Laboratory accelerator. With this measurement, the team has significantly improved the precision of this rate for stellar modeling. Bucher says, "We've studied its impact on the resulting stellar abundance pattern predictions, helping to identify the signature of the universe's elusive first generation of stars and their supernovae."
Contact: Brian Bucher (925) 422-7686 (bucher3@llnl.gov).

New Research Could Enable More Efficient Optics

In a research paper featured on the cover of the August 7, 2015, issue of *Physical Chemistry Chemical Physics*, a Livermore team provides new insight into specific factors that determine the absorption characteristics of copper complexes. The results demonstrate that conventional interpretations based on the ligand field theory—a staple concept in inorganic chemistry—are insufficient for capturing the full characteristics of the absorption profile. Instead, the team matched computational simulation results with experimental spectroscopic data to identify how specific spectral characteristics are triggered by the dynamics of the surrounding chemical environment.

"These results are a first step toward creating optically tunable materials for filters and for energy-efficient 'smart window' technologies. They also could help us better understand the role of metal–ligand complexes in photobiology," says Livermore's Roger Qiu, lead author of the paper.

The new research also demonstrates the power of combining the Laboratory's experimental and quantum chemistry simulation capabilities to tackle challenging scientific questions. This work is part of a project funded the Laboratory Directed Research and Development Program aimed at controlling the absorption characteristics of transition metal-ligand complexes for optical filter applications in high-power laser systems.
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Exposing the Strength of Beryllium

A team of scientists from Lawrence Livermore and the Russian Federal Nuclear Center-All-Russian Research Institute of Experimental Physics (RFNC-VNIIEF) has shown that at extreme conditions, beryllium has very little strength and most models overpredict its material strength. According to Marc Henry de Frahan, the lead author of a recent paper published on the cover of the *Journal of Applied Physics*, this finding has implications for scientists working with technology where beryllium is subject to extreme pressures and strain rates.

In the experiments, a piece of high explosive (HE) was detonated near the beryllium. The team imposed a sinusoidal ripple pattern on the beryllium samples. When the expanding HE products load up against the target, the target accelerates. The low-density gas pushes against the higher density metal, making the interface between the two materials Rayleigh–Taylor unstable, and the ripples grow in amplitude as the target accelerates. The ripple growth is limited by the strength of the beryllium. X-ray images of the side of the target showed the height of the ripples at some time after the HE loading occurred. Velocimetry measurements of the target showed its acceleration profile.

Because the researchers devised the initial ripple amplitude and measured the acceleration, they could infer the strength of the material using strength-model simulations. The experiment helped determine the effect of strength, which can refine the performance of various strength models.
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Scientists Discover Jupiter-Like Planet

Lawrence Livermore scientists, as part of an international team, have discovered the most Jupiter-like planet ever seen in a young star system. Using a new advanced adaptive-optics device on the Gemini Planet Imager (GPI)—located on the Gemini South Telescope in Chile—the team captured an image of the planet. Called 51 Eridani b, the planet could help scientists discover how Jupiter and other gas giants form and influence their planetary systems. Since a planet's luminosity is a function of age, mass, and initial conditions, luminosity can provide insight into the planet's formation, according to former Livermore researcher Bruce Macintosh of Stanford University, who was the lead author on a paper appearing in the August 14, 2015, edition of *Science*.

GPI—whose Livermore-developed adaptive optics are some of the most sophisticated in the world— was designed specifically for discovering and analyzing faint, young planets orbiting bright stars. The 51 Eridani b star is considered young—only 20 million years old and about twice the mass of Jupiter. When planets similar to 51 Eridani b coalesce, material falling into the planet releases energy and heats it up. Over the next 100 million years, these planets radiate that energy away, mostly as infrared light. Using GPI, astronomers observed the planet's characteristics, which seem to suggest what Jupiter was like in its infancy. Livermore's scientific involvement and technical support of GPI is led by S. Mark Ammons and funded by the Laboratory Directed Research and Development Program. Laboratory engineers Lisa Poyneer, David Palmer, and Brian Bauman made critical contributions to GPI's design.
Contact: S. Mark Ammons (925) 422-2102 (ammons1@llnl.gov).

Abstract

Advancing Next-Generation Rockets and the Engines that Power Them

Livermore researchers are developing new simulation tools and techniques to make possible cost-effective rocket-engine and launch-vehicle designs for national security and scientific exploration. These simulation tools promise to significantly reduce the time, cost, and risk of bringing new space-technology designs to realization. Livermore engineers and scientists are also creating and applying additive-manufacturing tools and techniques for space-technology applications to enable faster and cheaper routine production of complex parts with unique engineered attributes. Recently, Livermore engineers have worked on two efforts for the Defense Advanced Research Projects Agency (DARPA). For the first project, researchers conducted a series of simulations directed at evaluating a novel aerospike liquid-propellant rocket engine intended for DARPA's Next-Generation Rocket program. The simulations focused on the engine's injector performance, combustion characteristics, cooling system, thermal and structural characteristics, and altitude-compensating ability. The second effort used simulations for studying the thermal and structural response of a candidate launch-vehicle design for DARPA's proposed medium-lift-capacity XS-1 space plane.

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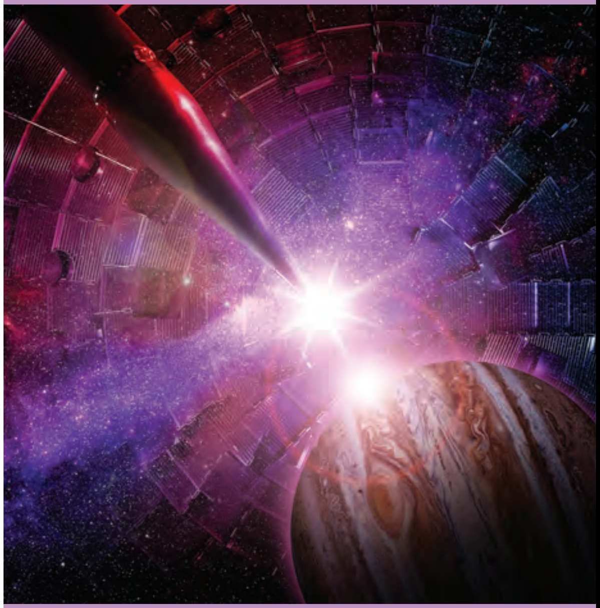
Smashing Science



Dynamic compression experiments shed light on matter's more extreme states.

Also in December

• Ocean salinity is proving a sensitive indicator of changing global rainfall patterns.

• X-ray free-electron lasers are improving understanding of the structure and dynamics of difficult-to-image proteins.

• Livermore scientists are developing a new microcapsule technology to control the capture and release of carbon dioxide emissions from coal-fired power plants.

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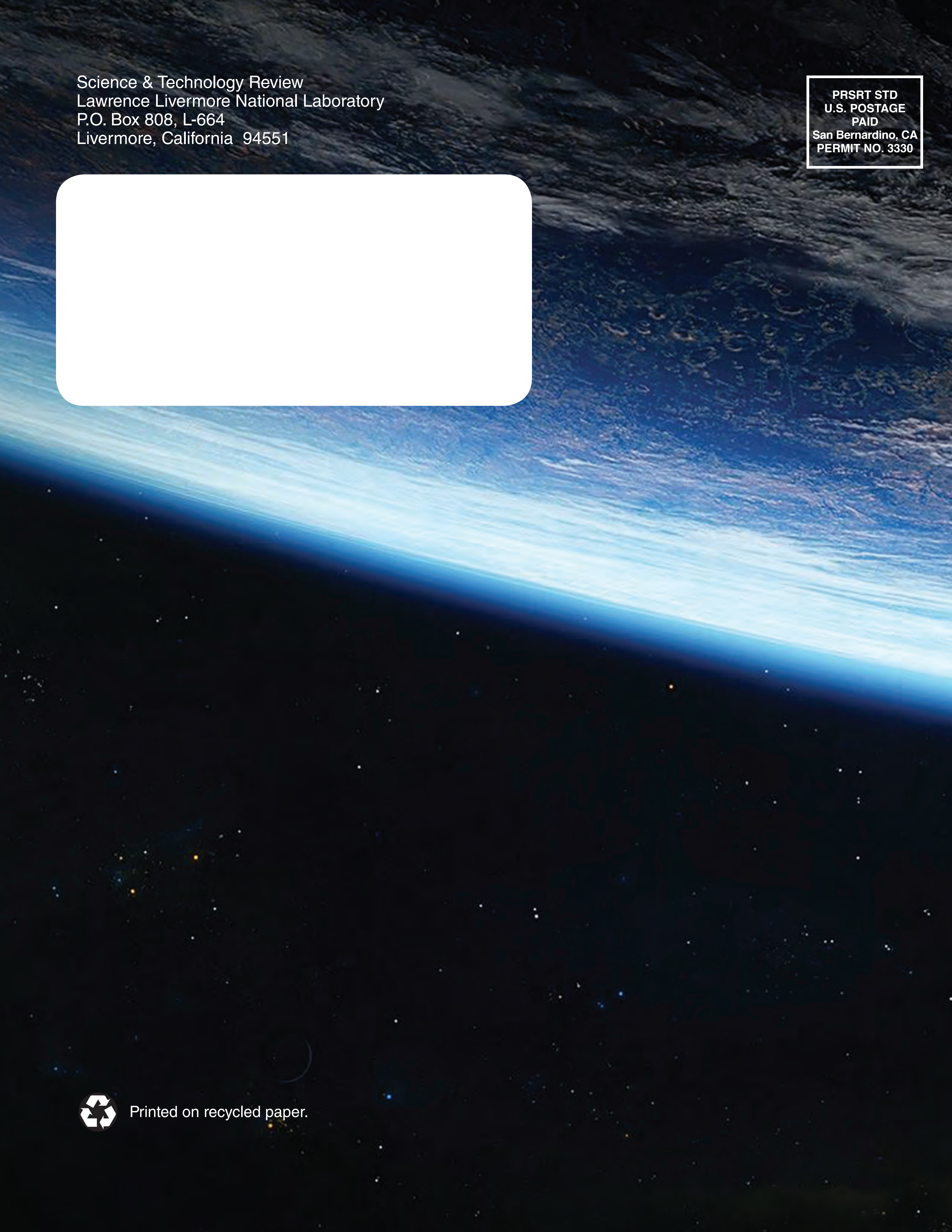

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